SUPPLEMENTARY INFORMATION

Fig. S1. Examples of raw chromatograms for lipidomics, serum metabolomics and urine metabolomics.

Fig. S2. Weight and creatinine levels of control and irradiated mice from each group.

Fig. S3. Expanded multivariate data analysis and PCA score plots for days 1 and 7, including control groups.

Fig. S4. Metabolites identified through serum metabolomics. Metabolites that showed statistically significant changes between the equidose exposures at day 1 included l-tyrosine, uric acid, taurine, pyroglutamic acid, l-carnitine, sphinganine-1-phosphate and succinic acid. Only sphinganine-1-phosphate remained perturbed between the two equidose exposures at day 7. Control vs. 1 Gy neutron irradiated groups also showed statistical significance for l-tyrosine, l-glutamic acid, uric acid, taurine, citric acid, pyroglutamic acid and l-carnitine at day 1. Overall, a generalized downregulation of the metabolites is seen at day 1 after 1 Gy neutron irradiation, except for l-carnitine levels, which are higher.

Fig. S5. Metabolites from urine and serum metabolomics together with lipidomics, which were utilized for the construction of the ROC curves; and heatmap depiction of patterns of change between 1 Gy exposures at days 1 and 7 postirradiation.

Table S1. Chromatographic and mass spectrometry details on the experiments.

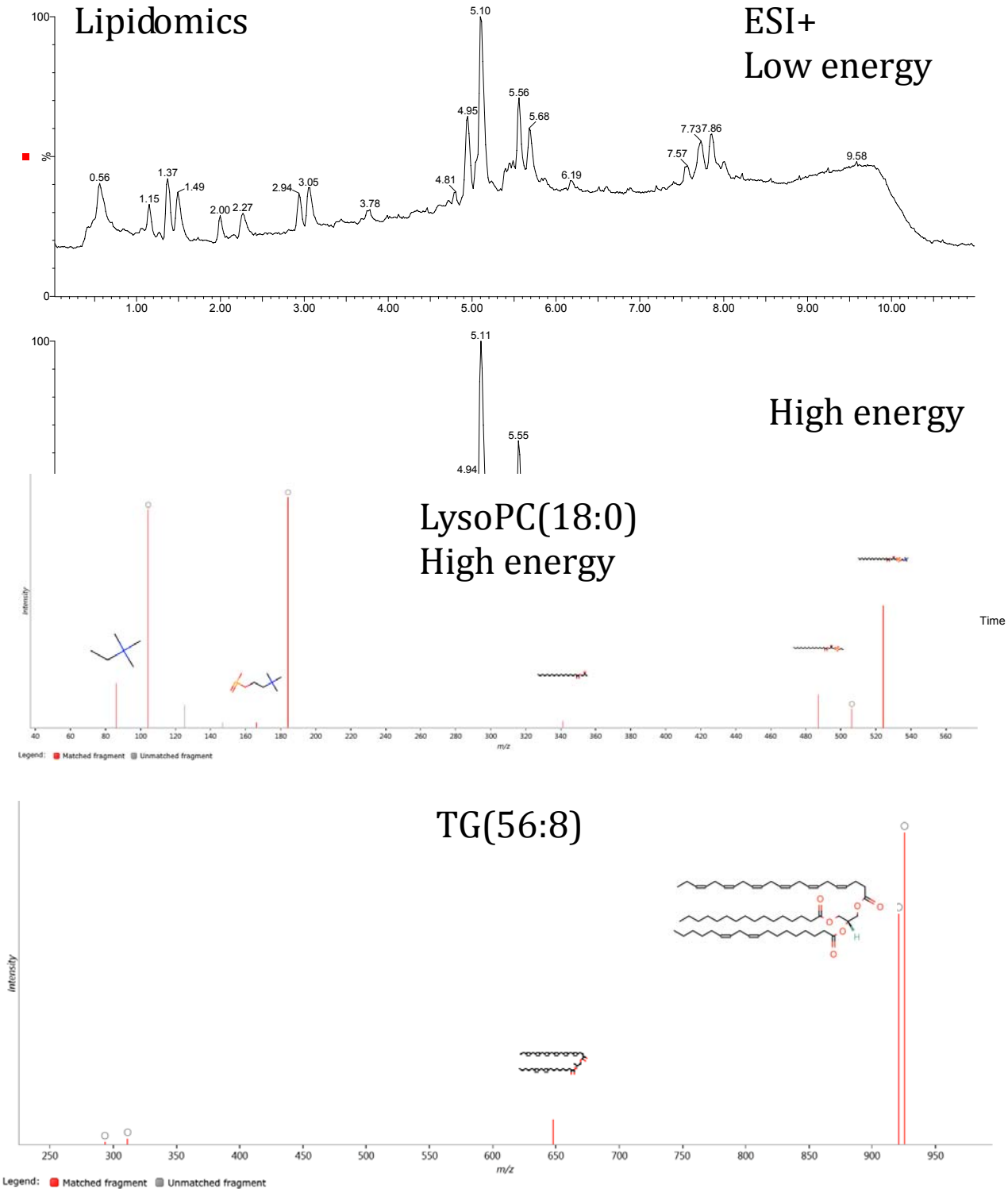
Table S2. Mean values of normalized relative abundance urine metabolomics data.

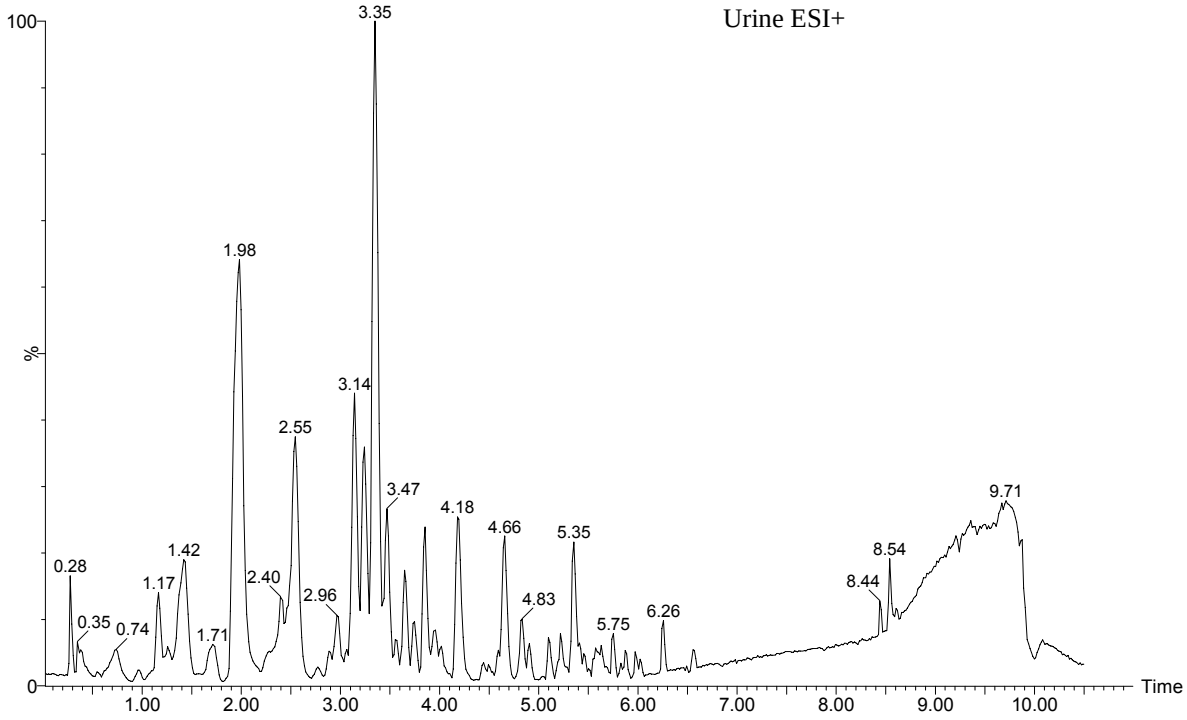
Table S3. Mean values of normalized relative abundance of serum metabolomics data.

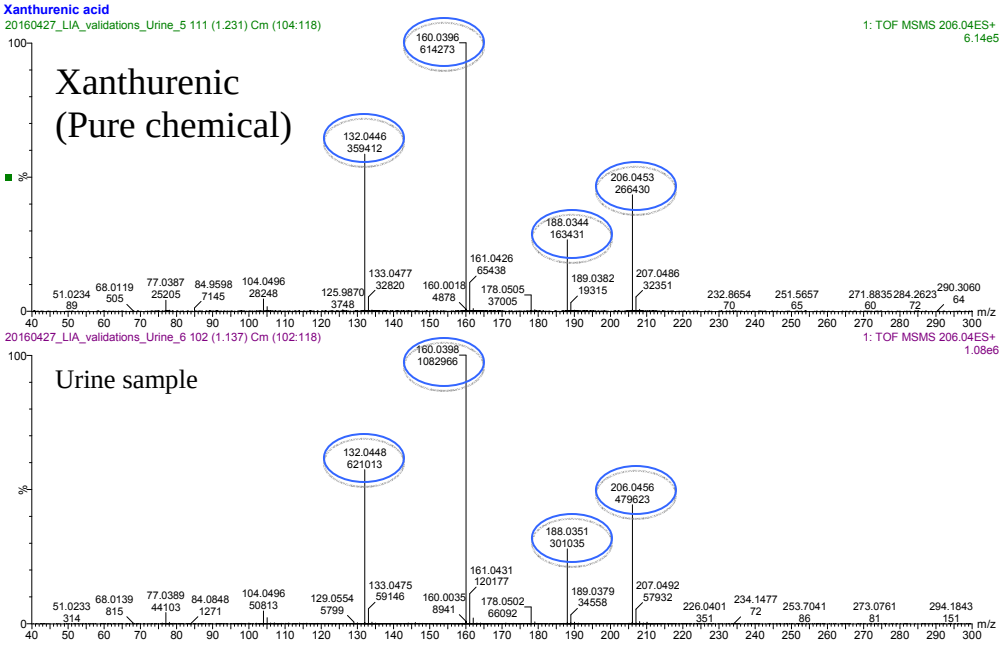
Table S4. Mean values of normalized relative abundance of serum lipidomics data.

Table S5. AUC values of each metabolite from individual ROC curves.

Supplementary Fig. S1




Urine ESI+
100
%
0
Time
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
9.00
10.00
3.35
1.98
3.14
2.55
3.47
4.18
4.66
5.35
9.71
8.54
1.42
1.17
2.40
2.96
4.83
8.44
6.26
5.75
0.28
0.35
0.74
1.71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6.14e5
Xanthurenic
(Pure chemical)
160.0396 614273
132.0446 359412
206.0453 266430
188.0344 163431
161.0426 65438
133.0477 32820
189.0382 19315
207.0486 32351
160.0018 4878
178.0505 37005
125.9870 3748
51.0234 89
68.0119 505
77.0387 25205
84.9598 7145
104.0496 28248
232.8654 70
251.5657 65
271.8835 60
284.2623 72
290.3060 64
20160427_LIA_validations_Urine_6 102 (1.137) Cm (102:118)
1: TOF MSMS 206.04ES+
1.08e6
Urine sample
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206.0456 479623
188.0351 301035
161.0431 120177
133.0475 59146
189.0379 34558
207.0492 57932
160.0035 8941
178.0502 66092
129.0554 5799
51.0233 314
68.0139 815
77.0389 44103
84.0848 1271
104.0496 50813
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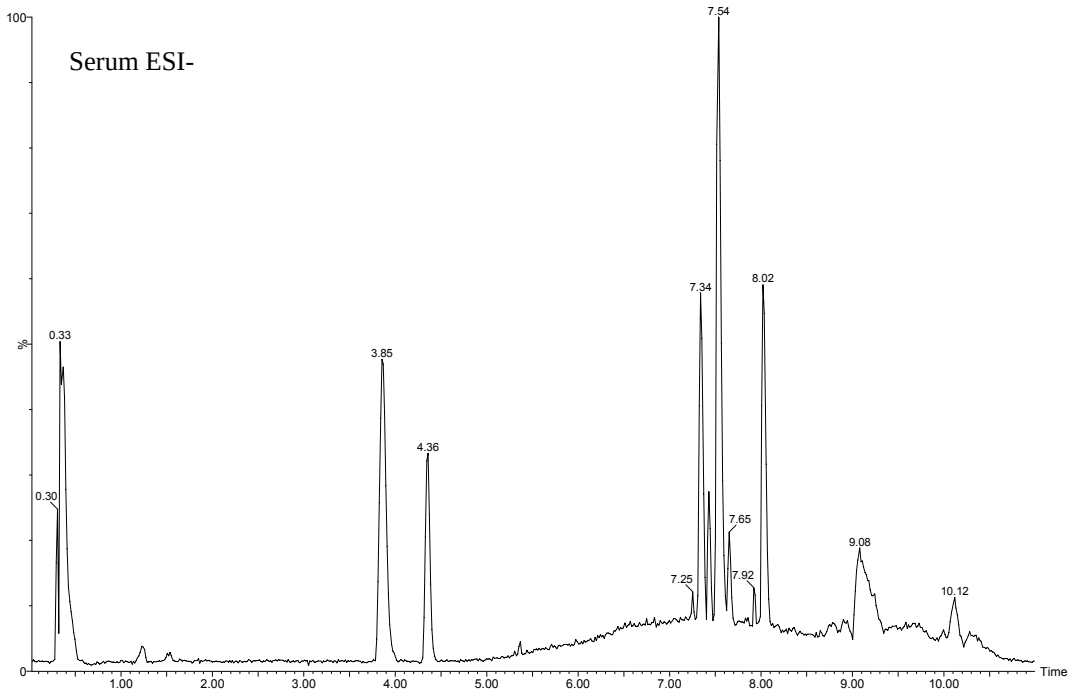
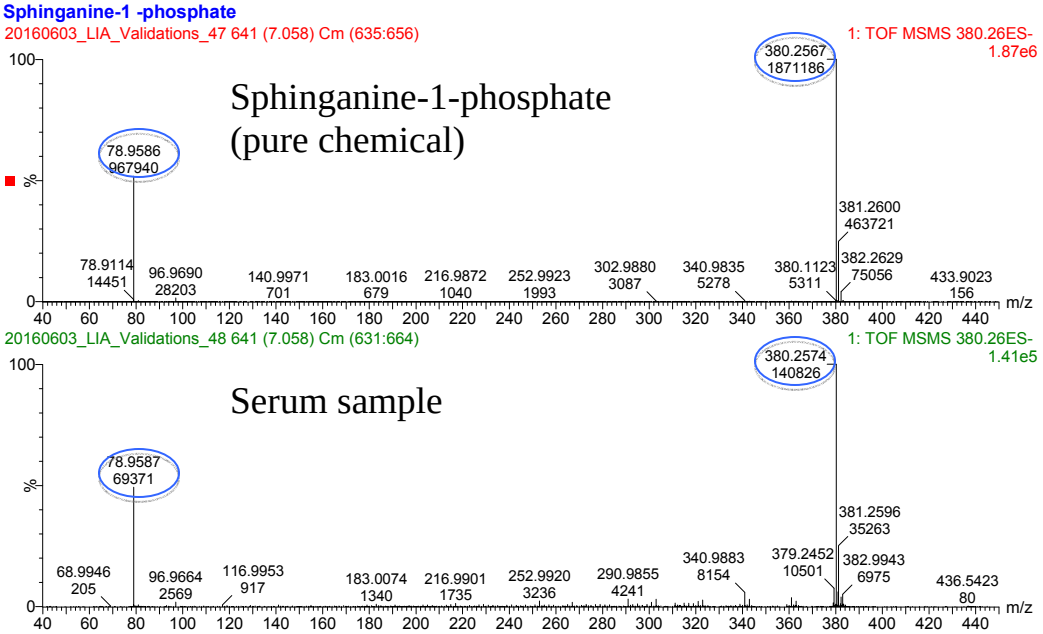
253.7041 86
273.0761 81
294.1843 151
m/z


Serum ESI-
100
%
0
0.33
0.30
3.85
4.36
7.34
7.54
8.02
7.65
7.25
7.92
9.08
10.12
1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
9.00
10.00
Time


Sphinganine-1 -phosphate
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1: TOF MSMS 380.26ES-
1.87e6
Sphinganine-1-phosphate
(pure chemical)
380.2567
1871186
78.9586
967940
381.2600
463721
382.2629
75056
78.9114
14451
96.9690
28203
140.9971
701
183.0016
679
216.9872
1040
252.9923
1993
302.9880
3087
340.9835
5278
380.1123
5311
433.9023
156
m/z
20160603_LIA_Validations_48 641 (7.058) Cm (631:664)
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1.41e5
Serum sample
380.2574
140826
78.9587
69371
381.2596
35263
382.9943
6975
68.9946
205
96.9664
2569
116.9953
917
183.0074
1340
216.9901
1735
252.9920
3236
290.9855
4241
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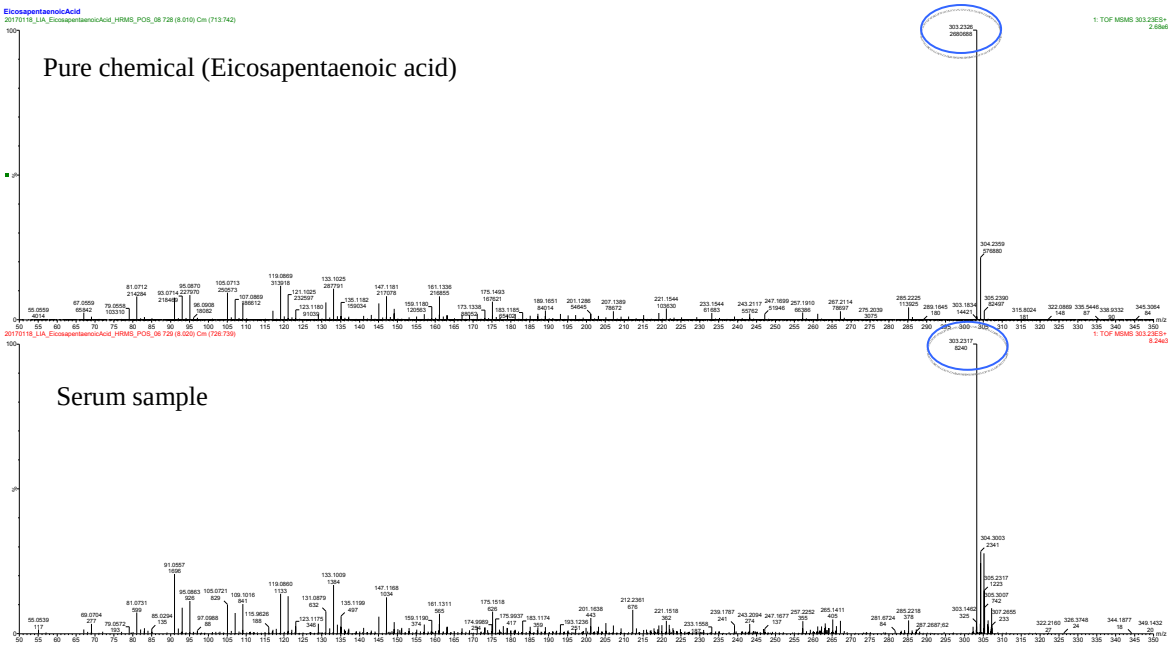
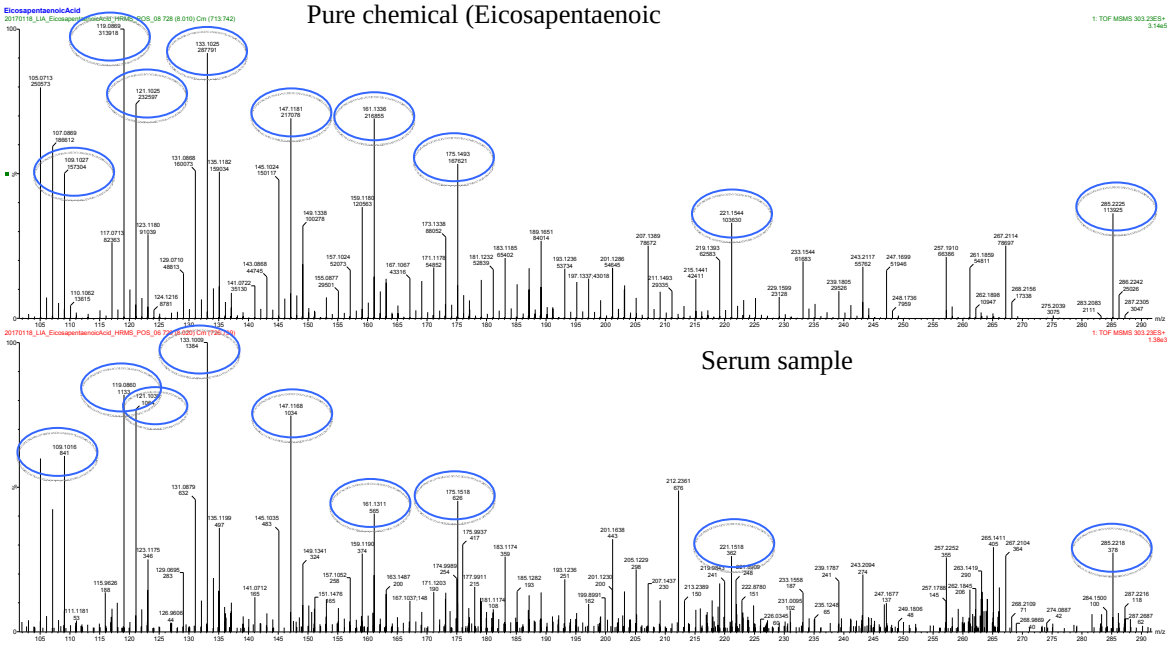
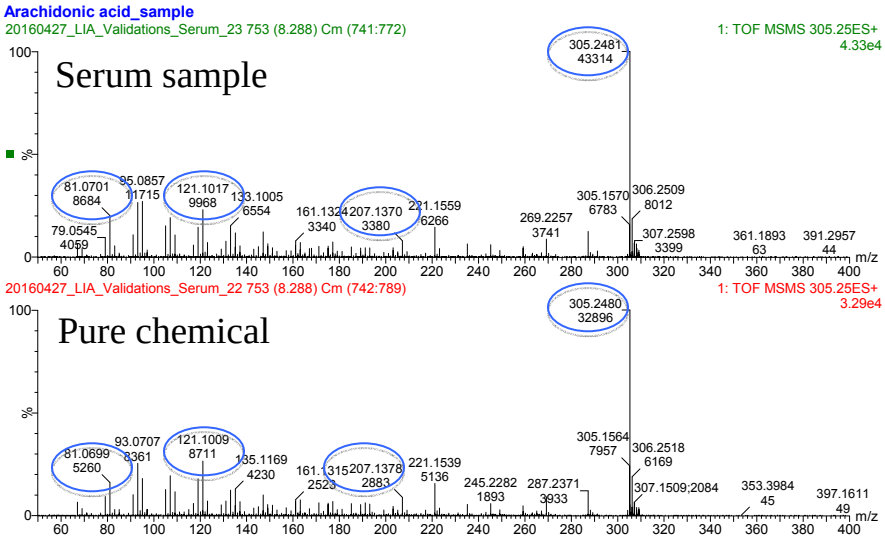
8154
379.2452
10501
436.5423
80
m/z


EicosapentaenoicAcid
Pure chemical (Eicosapentaenoic acid)
Serum sample

Zoom in


EicosapentaenoicAcid
Pure chemical (Eicosapentaenoic
Serum sample


Arachidonic acid_sample
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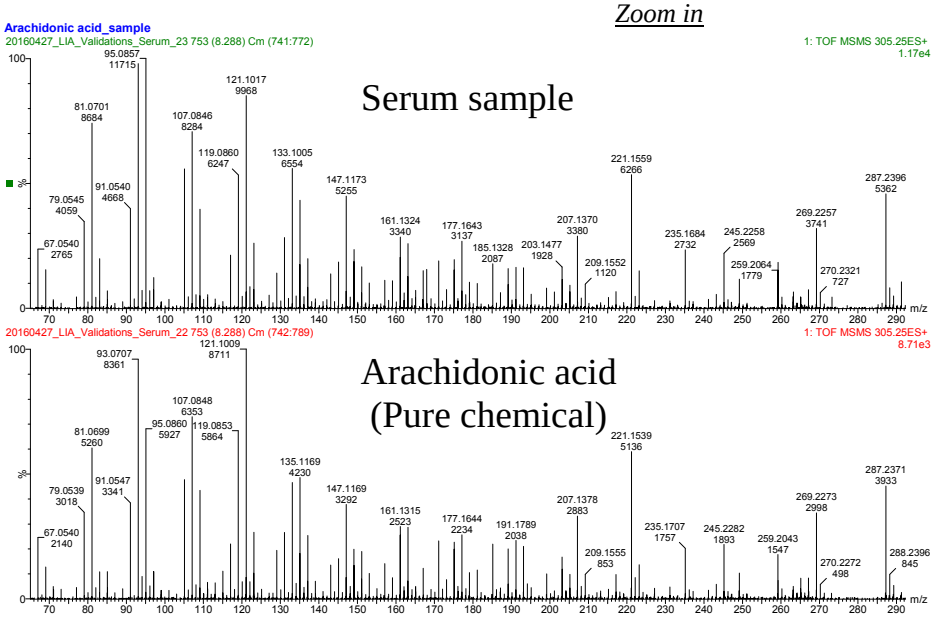
1: TOF MSMS 305.25ES+
4.33e4
Serum sample
305.2481 43314
81.0701 8684
95.0857 11715
121.1017 9968
133.1005 6554
161.1324 3340
207.1370 3380
221.1559 6266
269.2257 3741
305.1570 6783
306.2509 8012
307.2598 3399
79.0545 4059
361.1893 63
391.2957 44
20160427_LIA_Validations_Serum_22 753 (8.288) Cm (742:789)
1: TOF MSMS 305.25ES+
3.29e4
Pure chemical
305.2480 32896
81.0699 5260
93.0707 8361
121.1009 8711
135.1169 4230
161.1315 2523
207.1378 2883
221.1539 5136
245.2282 1893
287.2371 3933
305.1564 7957
306.2518 6169
307.1509;2084
353.3984 45
397.1611 49
m/z

Zoom in


Arachidonic acid_sample
20160427_LIA_Validations_Serum_23 753 (8.288) Cm (741:772)
1: TOF MSMS 305.25ES+
1.17e4
Serum sample
95.0857 11715
121.1017 9968
81.0701 8684
107.0846 8284
119.0860 6247
133.1005 6554
147.1173 5255
221.1559 6266
287.2396 5362
79.0545 4059
91.0540 4668
161.1324 3340
177.1643 3137
207.1370 3380
269.2257 3741
67.0540 2765
185.1328 2087
203.1477 1928
235.1684 2732
245.2258 2569
209.1552 1120
259.2064 1779
270.2321 727
20160427_LIA_Validations_Serum_22 753 (8.288) Cm (742:789)
1: TOF MSMS 305.25ES+
8.71e3
Arachidonic acid
(Pure chemical)
121.1009 8711
93.0707 8361
107.0848 6353
95.0860 5927
119.0853 5864
81.0699 5260
221.1539 5136
135.1169 4230
287.2371 3933
91.0547 3341
147.1169 3292
207.1378 2883
269.2273 2998
79.0539 3018
161.1315 2523
177.1644 2234
191.1789 2038
235.1707 1757
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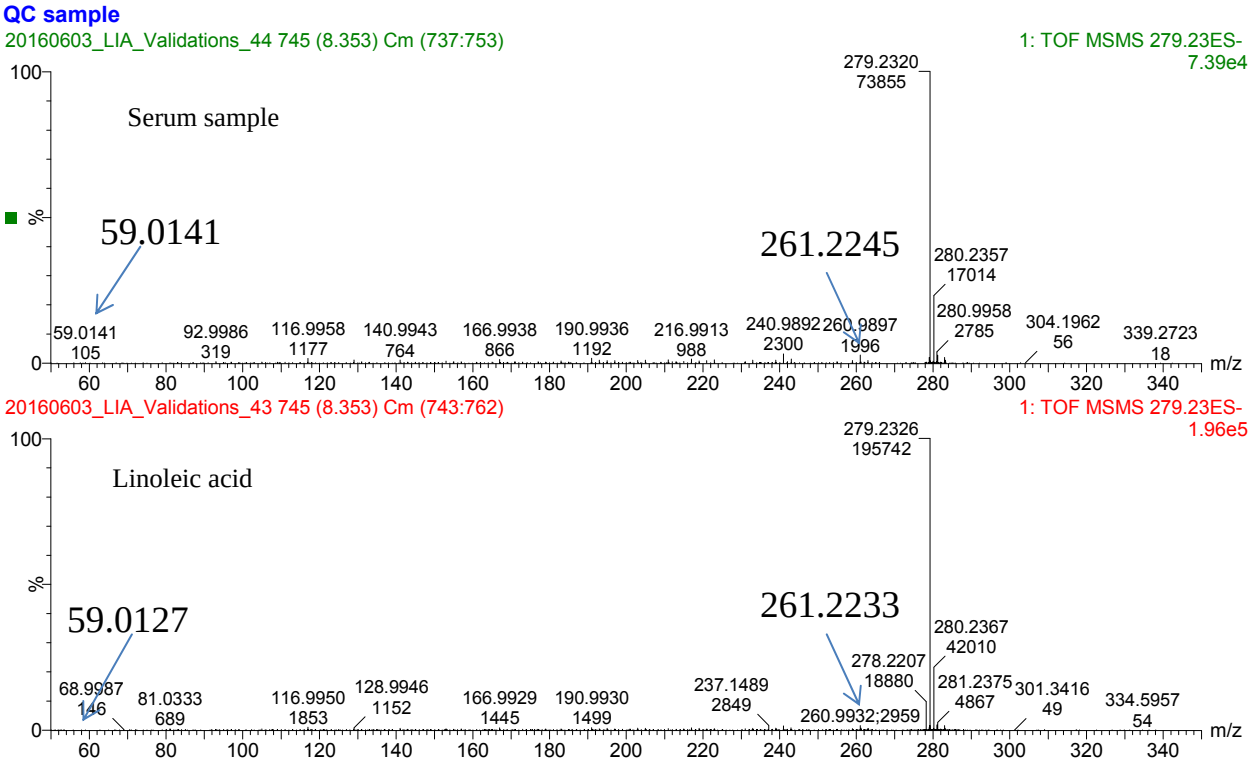
259.2043 1547
67.0540 2140
209.1555 853
270.2272 498
288.2396 845
m/z


QC sample
20160603_LIA_Validations_44 745 (8.353) Cm (737:753)
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7.39e4
Serum sample
59.0141
261.2245
279.2320
73855
280.2357
17014
280.9958
2785
304.1962
56
339.2723
18
59.0141
105
92.9986
319
116.9958
1177
140.9943
764
166.9938
866
190.9936
1192
216.9913
988
240.9892
2300
260.9897
1996
m/z
20160603_LIA_Validations_43 745 (8.353) Cm (743:762)
1: TOF MSMS 279.23ES-
1.96e5
Linoleic acid
59.0127
261.2233
279.2326
195742
280.2367
42010
278.2207
18880
281.2375
4867
301.3416
49
334.5957
54
68.9987
146
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689
116.9950
1853
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1152
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1445
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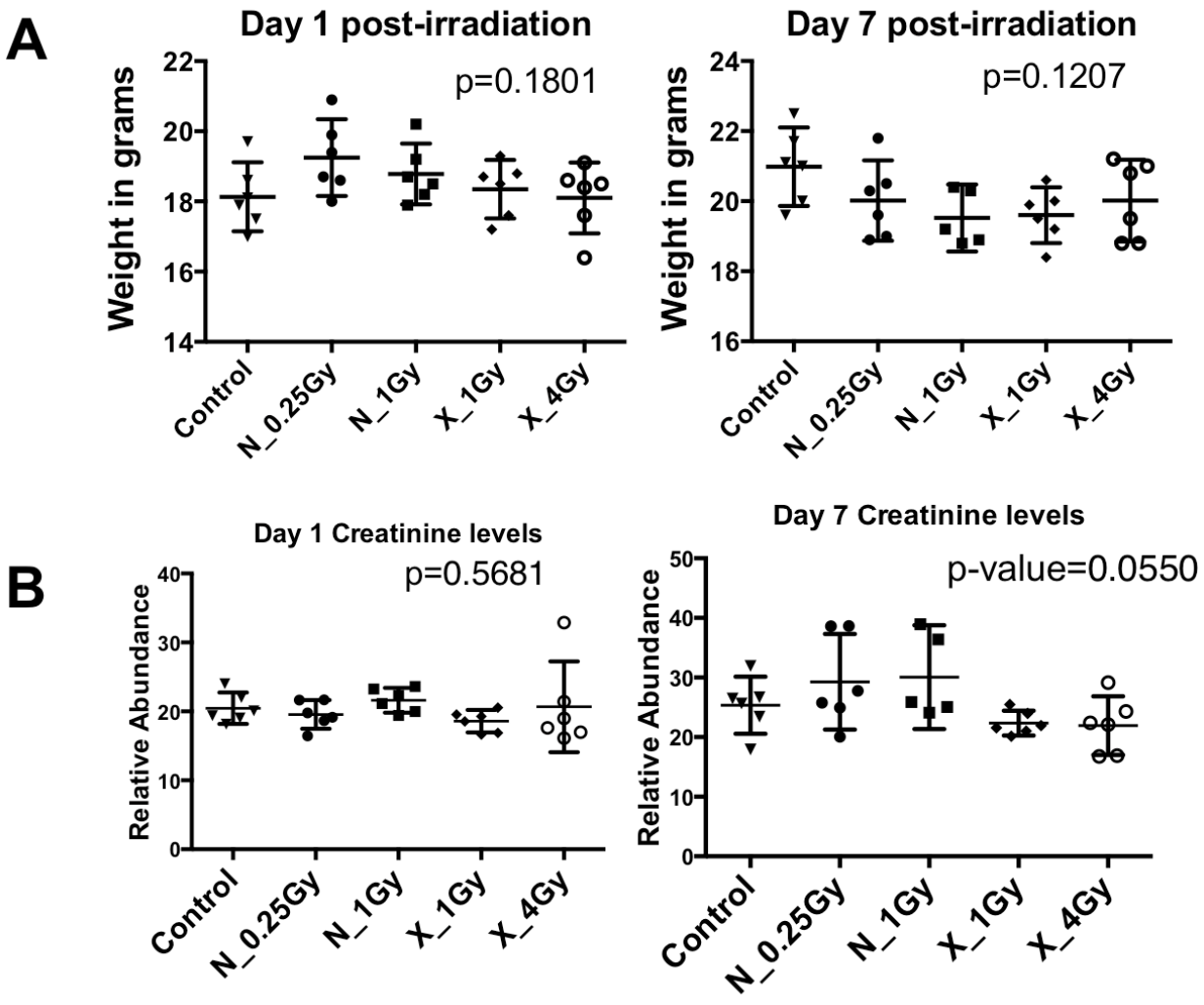
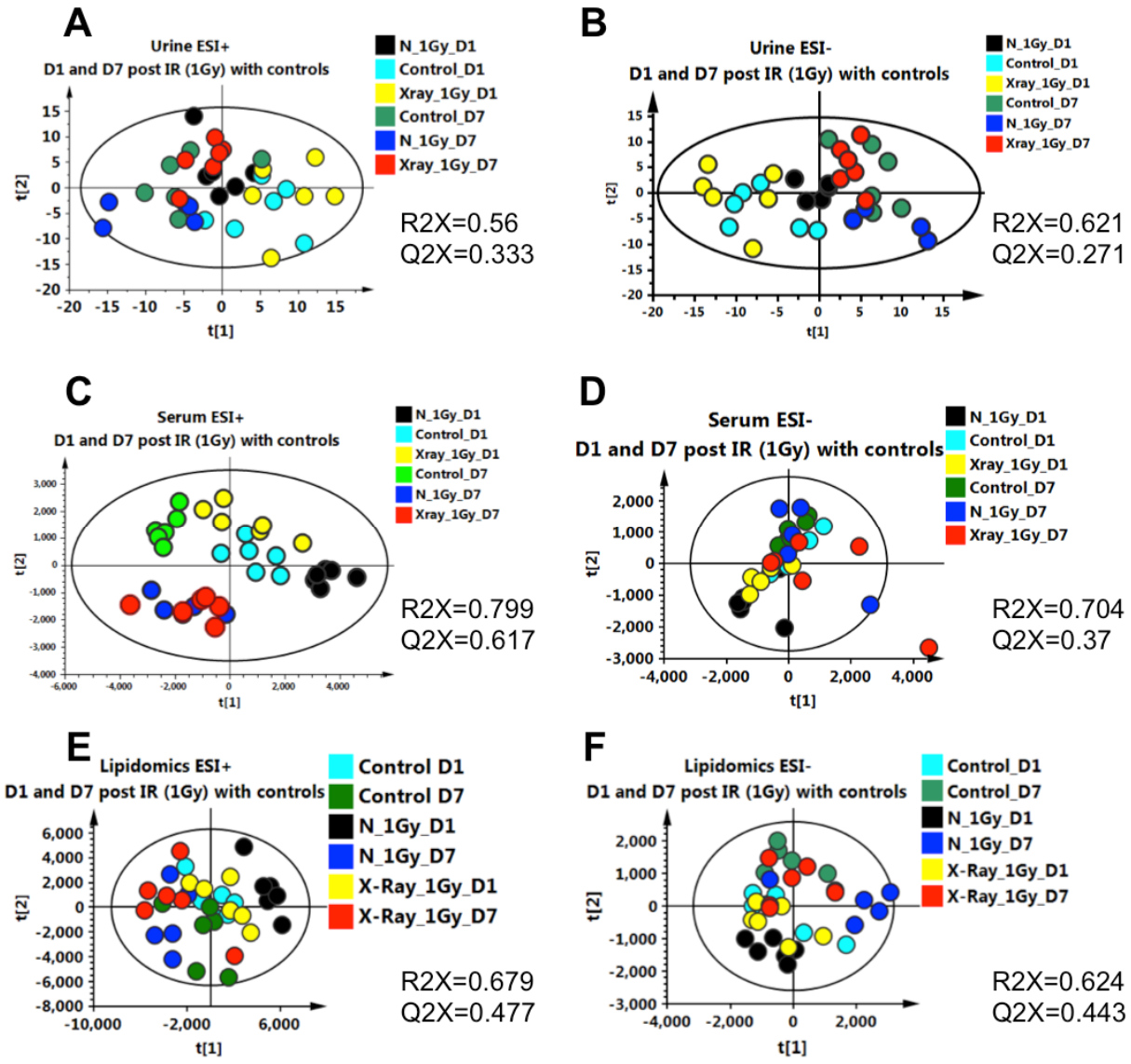
1499
237.1489
2849
260.9932;2959
m/z

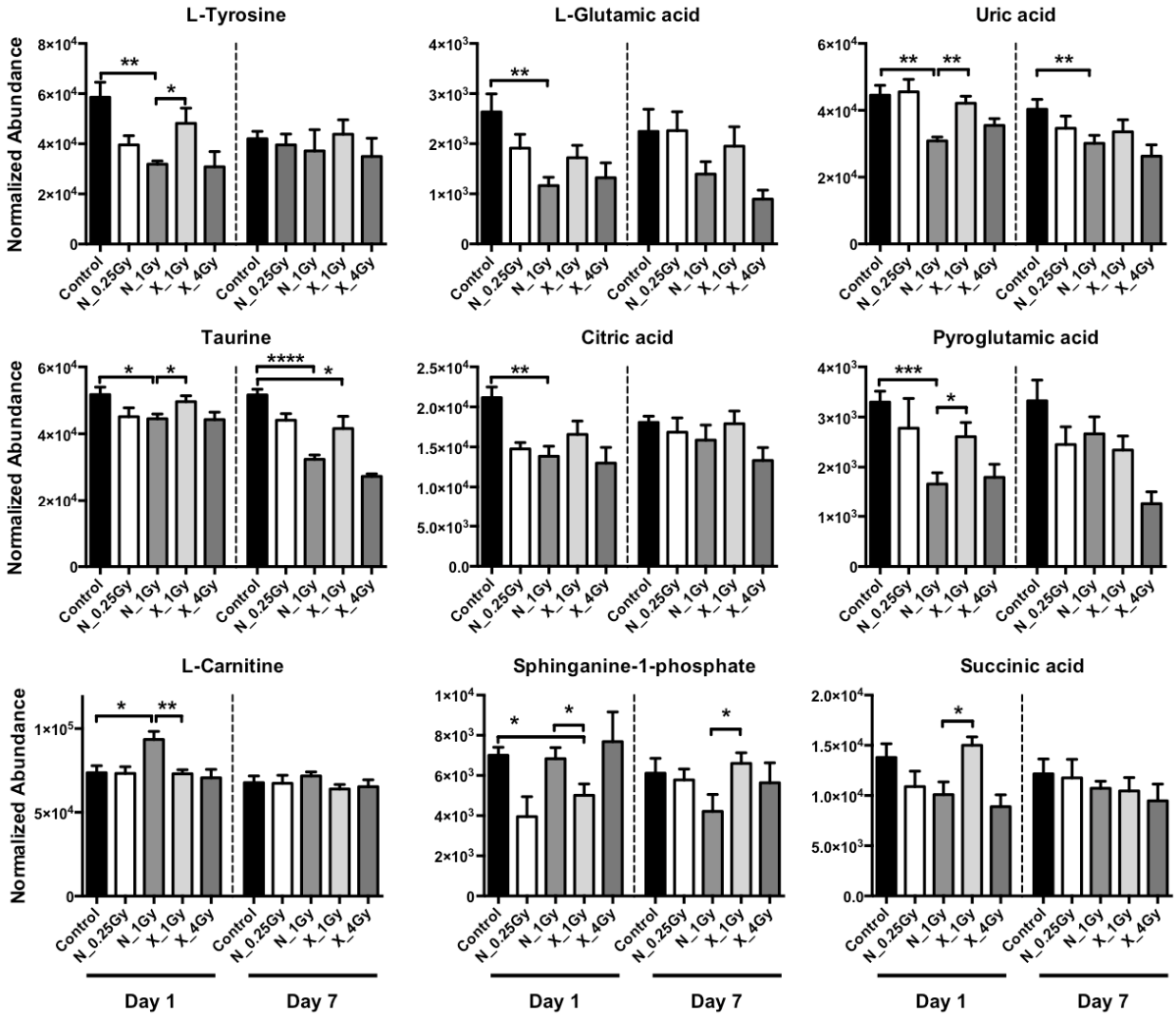
Supplementary Fig. S2



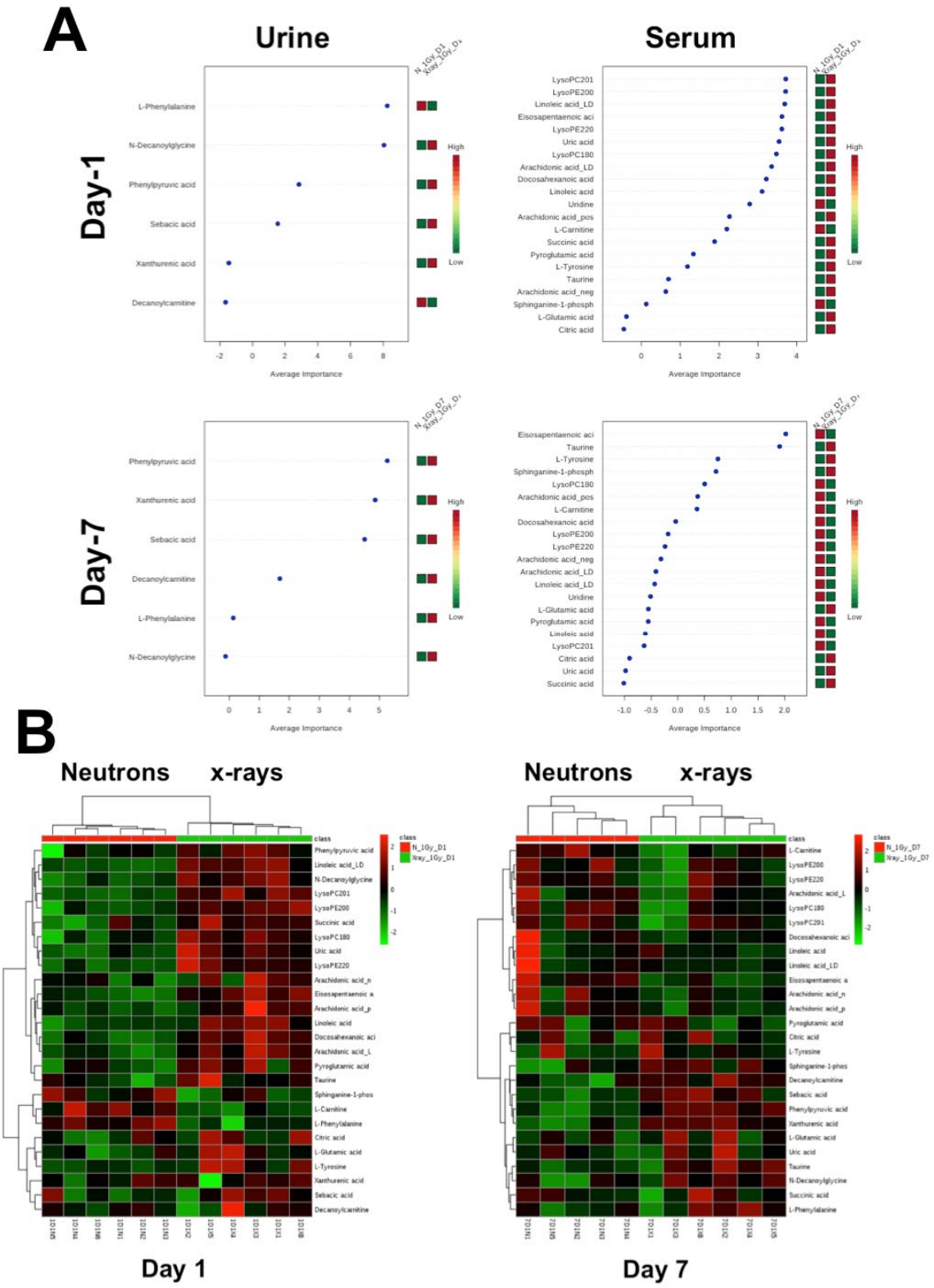
Supplementary Fig. S3



Supplementary Fig. S4



Supplementary Fig. S5



Supplementary Table S1: Chromatographic and mass spectrometry details on the experiments.

Chromatographic conditions for Global Urine Metabolomics

Step	Time (min)	Flow (mL/min)	% A	% B	Curve Initial
1	Initial	0.5	95	5	Initial
2	0.5	0.5	95	5	6
3	4	0.5	80	20	6
4	8	0.5	5	95	6
5	9	0.5	5	95	6
6	9.1	0.5	95	5	6
7	10.5	0.5	95	5	6

Solvent A: Water + 0.1% Formic acid
Solvent B: Acetonitrile + 0.1% Formic acid

Chromatographic conditions for Global Serum Metabolomics

Step	Time (min)	Flow (mL/min)	% A	% B	Curve Initial
1	Initial	0.5	95	5	Initial
2	0.5	0.5	95	5	6
3	4	0.5	80	20	6
4	8	0.5	5	95	6
5	9	0.5	5	95	6
6	9.5	0.5	95	5	6
7	11	0.5	95	5	6
					6

Solvent A: Water + 0.1% Formic acid
Solvent B: Acetonitrile + 0.1% Formic acid

Chromatographic conditions for Global Lipidomics

Step	Time (min)	Flow (mL/min)	% C	% D	Curve Initial
1	Initial	0.45	60	40	Initial
2	0.5	0.45	60	40	6
3	8	0.45	0	100	6
4	8.5	0.45	0	100	6
5	9	0.45	60	40	6
6	11	0.45	60	40	6

Solvent C: 50:50 Water:Acetonitrile +0.1% Formic acid + 10mM HCOONH4
Solvent D: 90:10 Isopropanol:Acetonitrile + 0.1% Formic acid + 10mM HCOONH4

Other parameteres

Instrument	Parameter	Urine Metabolomics	Serum Metabolomics	Lipidomics
Autosampler	Injection volume µL	2	2	2
Column Oven	Temperature °C	40	60	65
MS	Capillary Voltage kV	2.5	2.5	2.8
	Cone Voltage V	50	50	30
	Source Temp °C	120	120	120
	Desolvation Temp °C	500	500	500
	Cone Gas Flow (L/Hr)	25	25	25
	Desolvation Gas (L/Hr)	1000	1000	1000
	Collision Energy V	6	6	6

Supplementary Table S2: Mean values of **normalized relative abundance** urine metabolomics data.

					Day 1						
Metabolite	**Control**	**SEM**	**N_0.25Gy**	**SEM**	**N_1Gy**	**SEM**	**x-ray_1Gy**	**SEM**	**x-ray_4Gy**	**SEM**	**ANOVA p-value**
L-Phenylalanine	0.068	0.006	0.068	0.013	0.089	0.004	0.059	0.006	0.041	0.015	0.0072
Phenylpyruvic acid	0.160	0.010	0.169	0.014	0.121	0.020	0.178	0.013	0.165	0.024	0.1843
Xanthurenic acid	1.476	0.117	1.771	0.054	1.571	0.115	1.552	0.201	1.924	0.278	0.356
N-Decanoylglycine	0.087	0.013	0.054	0.008	0.028	0.007	0.098	0.011	0.080	0.022	0.0067
Decanoylcarnitine	0.016	0.004	0.024	0.004	0.020	0.001	0.021	0.003	0.017	0.004	0.5054
Sebacic acid	0.603	0.101	0.571	0.087	0.599	0.184	0.758	0.117	0.742	0.162	0.4958
					Day 7						
Metabolite	**Control**	**SEM**	**N_0.25Gy**	**SEM**	**N_1Gy**	**SEM**	**x-ray_1Gy**	**SEM**	**x-ray_4Gy**	**SEM**	**ANOVA p-value**
L-Phenylalanine	0.106	0.013	0.083	0.014	0.101	0.013	0.131	0.022	0.111	0.010	0.2556
Phenylpyruvic acid	0.090	0.021	0.106	0.017	0.107	0.014	0.208	0.012	0.274	0.025	<0.0001
Xanthurenic acid	1.343	0.123	1.355	0.281	0.958	0.179	1.954	0.105	1.586	0.201	0.0204
N-Decanoylglycine	0.034	0.010	0.030	0.010	0.028	0.012	0.050	0.007	0.060	0.009	0.1073
Decanoylcarnitine	0.022	0.002	0.015	0.004	0.016	0.003	0.025	0.002	0.022	0.003	0.1312
Sebacic acid	0.299	0.104	0.228	0.089	0.155	0.036	0.384	0.097	0.351	0.136	0.1494

Supplementary Table S3: Mean values of **normalized relative abundance of** serum metabolomics data.

	Day 1										
Metabolite	**Control**	**SEM**	**N_0.25Gy**	**SEM**	**N_1Gy**	**SEM**	**x-ray_1Gy**	**SEM**	**x-ray_4Gy**	**SEM**	**ANOVA p-value**
L-Tyrosine	58550.50	6012.39	39485.29	3701.88	31902.34	1291.87	48169.42	6045.82	30863.71	6053.79	0.0027
L-Glutamic acid	2634.62	359.66	1911.09	276.02	1163.41	168.24	1722.78	246.28	1322.91	295.81	0.0081
Taurine	51710.40	2271.59	45146.03	2641.91	44513.84	1419.72	49627.45	1762.81	44209.53	2214.84	0.0589
Succinic acid	13785.22	1375.16	10899.12	1523.78	10092.03	1273.85	15011.19	836.10	8888.91	1192.17	0.0103
L-Carnitine	73673.91	4143.59	73281.80	4005.70	93535.49	4779.13	73006.85	2486.55	70613.88	5008.89	0.0039
Pyroglutamic acid	3298.57	215.73	2778.25	592.43	1664.90	222.19	2609.38	282.56	1798.25	259.58	0.0124
Eisosapentaenoic acid	3364.37	171.97	3036.26	680.23	995.95	264.76	3702.40	382.99	2597.29	232.66	0.0005
Linoleic acid	4719.98	974.12	3988.15	1301.36	984.07	207.35	3160.32	452.34	3109.29	886.56	0.0556
Arachidonic acid_neg	13161.06	1376.36	12475.65	1059.25	8501.81	786.83	11021.83	1311.47	9584.38	506.93	0.0248
Arachidonic acid_pos	27450.37	1194.02	26474.13	933.46	19702.77	571.15	25207.13	1749.77	24988.73	668.90	0.0005
Uric acid	44507.15	2985.00	45528.37	3744.36	30891.36	1115.49	42132.87	2086.64	35463.01	2037.01	0.0015
Sphinganine-1-phosphate	7001.32	403.21	3957.37	987.11	6840.94	549.75	5014.79	567.38	7688.26	1475.71	0.0349
Citric acid	21161.26	1323.04	14770.52	791.02	13846.92	1239.02	16567.89	1665.64	12980.98	1975.54	0.0043

	Day 7										
Metabolite	**Control**	**SEM**	**N_0.25Gy**	**SEM**	**N_1Gy**	**SEM**	**x-ray_1Gy**	**SEM**	**x-ray_4Gy**	**SEM**	**ANOVA p-value**
L-Tyrosine	42005.70	2959.13	39545.10	4360.89	37171.23	8469.29	43822.36	5762.46	34980.42	7241.09	0.8268
L-Glutamic acid	2243.91	445.63	2262.57	375.59	1395.63	245.69	1953.28	383.70	895.72	178.86	0.0401
Taurine	51643.72	1677.00	44065.05	1965.51	32328.49	1310.68	41593.23	3609.94	27298.93	709.36	< 0.0001
Succinic acid	12157.51	1477.66	11765.78	1840.99	10725.13	693.48	10464.66	1324.92	9479.68	1657.11	0.7173
L-Carnitine	67768.78	3994.28	67378.99	4806.84	71766.52	2334.06	63993.15	2608.23	65301.36	4112.43	0.6867
Pyroglutamic acid	3325.74	413.55	2451.42	352.72	2664.51	341.98	2342.35	278.05	1272.37	235.72	0.0037
Eisosapentaenoic acid	5632.25	517.31	4637.31	582.72	7542.43	1240.34	3574.08	656.80	3667.64	378.39	0.0034
Linoleic acid	7532.85	1537.38	6101.22	584.86	7577.71	2889.56	5453.58	1024.31	3730.87	880.20	0.3471
Arachidonic acid_neg	16338.00	1439.90	15743.65	1714.96	21348.79	3830.68	15026.76	1473.06	15015.64	659.42	0.1843
Arachidonic acid_pos	34275.43	2110.79	32604.61	1881.91	42037.61	4176.10	32455.54	1957.72	34852.65	1556.90	0.0689
Uric acid	40326.22	2959.95	34625.43	3670.07	30143.51	2369.49	33550.18	3612.17	26259.42	3397.66	0.0628
Sphinganine-1-phosphate	6113.87	739.79	5781.12	543.08	4214.70	842.71	6603.15	525.30	5635.85	991.57	0.2907
Citric acid	18048.36	769.33	16846.05	1787.00	15859.23	1882.92	17910.34	1575.76	13331.74	1596.21	0.2082

Supplementary Table S4: Mean values of **normalized relative abundance of** serum lipidomics data.

		Day 1										
Metabolite	**Class**	**Control**	**SEM**	**N_0.25Gy**	**SEM**	**N_1Gy**	**SEM**	**x-ray_1Gy**	**SEM**	**x-ray_4Gy**	**SEM**	**ANOVA p-value**
Linoleic acid	Fatty acid	16256.49	2381.21	12804.20	3531.59	5131.81	213.57	11404.58	759.43	9037.53	1852.35	0.0002
Docosahexanoic acid	Fatty acid	57419.98	3523.20	55875.61	9296.89	31698.11	2011.51	48484.36	2554.37	47309.83	8214.32	0.0036
Arachidonic acid	Fatty acid	34937.51	3986.24	32325.25	6274.72	19251.23	1079.14	29305.07	1872.30	22292.79	2281.57	0.001
CE(18:2)	Cholesteryl ester	1271882.24	49002.38	1036686.71	135188.16	1051254.50	42148.57	1333225.18	40615.45	1297869.46	80423.51	0.0009
CE(18:3)	Cholesteryl ester	69635.30	4349.72	45444.99	11896.02	46321.29	2460.78	73553.68	5135.50	78147.30	8573.21	0.0008
CE(20:4)	Cholesteryl ester	1635493.98	109778.19	1449040.97	284952.61	1369097.79	71398.36	1828127.26	48628.67	1920138.45	124954.91	0.0019
CE(20:5)	Cholesteryl ester	291342.63	21283.42	180005.13	41217.73	176413.24	6712.33	325445.43	25396.05	357455.23	26100.59	<0.0001
CE(22:6)	Cholesteryl ester	1127582.87	61022.14	811655.18	195714.18	857370.19	51947.66	1194726.85	74333.00	1550071.15	202170.84	0.0004
LysoPC(18:0)	Lysophosphatidylcholine	1467391.90	50808.70	1475101.18	218298.51	1093845.89	79460.54	1514379.68	60952.71	1457499.38	124083.36	0.0221
LysoPC(20:1)	Lysophosphatidylcholine	9613.55	1104.27	6779.92	2516.36	3208.90	257.03	9315.92	756.80	6673.30	1658.99	0.0014
LysoPE(20:0)	Lysophosphatidylethanolamine	23537.64	1062.00	21711.10	3286.29	16282.20	870.99	22569.03	682.31	20628.74	1007.15	0.0017
LysoPE(22:0)	Lysophosphatidylethanolamine	13632.44	915.16	14835.44	2134.82	9971.34	450.58	15547.88	973.35	11527.90	822.25	0.0007
TG(52:1)	Triacylglycerol	125655.38	54429.40	42767.82	7610.75	38453.84	3277.38	67599.22	6354.96	72572.52	13097.05	0.0054
TG(52:3)	Triacylglycerol	1502171.10	110539.63	791410.45	183049.80	781347.83	79611.99	1386672.56	128923.19	1488159.33	291343.41	0.0028
TG(55:3)	Triacylglycerol	53115.68	4063.66	19589.00	6449.04	17020.83	5525.23	45313.56	5327.27	44879.56	13093.28	0.0041
TG(56:4)	Triacylglycerol	46333.57	9618.87	12235.77	13493.13	15360.80	6199.85	60741.13	9799.70	84446.27	20213.83	0.0005
TG(56:6)	Triacylglycerol	288167.12	35723.69	86792.36	46822.13	98780.06	15107.56	289769.24	31973.81	380356.24	58804.34	<0.0001
TG(56:8)	Triacylglycerol	732372.46	63798.43	273181.52	139439.75	279733.49	24060.26	689135.07	69695.67	853997.60	111542.41	<0.0001
TG(57:3)	Triacylglycerol	379167.96	25297.53	231508.33	35381.46	218208.08	21539.73	359453.09	25338.32	362288.98	68240.61	0.0071
TG(57:3)	Triacylglycerol	55274.56	4034.58	29226.10	12931.89	30334.48	2500.89	55118.70	5444.45	63146.76	5819.32	<0.0001
TG(57:4)	Triacylglycerol	338753.77	28731.56	219230.53	40222.88	206776.23	21747.96	332384.86	25870.32	319745.48	59725.91	0.0252
TG(58:10)	Triacylglycerol	109809.05	15089.12	27016.88	24629.85	29061.34	5084.13	101806.49	14870.22	152572.01	28818.37	<0.0001
TG(58:10)	Triacylglycerol	33357.70	4933.17	4526.26	8208.95	4131.13	1524.00	33691.04	5983.39	47419.59	10334.69	<0.0001
TG(58:3)	Triacylglycerol	118509.94	9123.77	61862.64	13134.85	61477.03	8616.63	112063.17	9769.78	117121.96	24875.19	0.0054
TG(58:4)	Triacylglycerol	108601.49	12533.56	58204.66	15775.12	56899.72	7425.11	102195.55	9731.24	106164.05	23508.84	0.0183
TG(58:8)	Triacylglycerol	107989.99	18769.20	24780.81	18544.82	35723.82	5325.40	100827.61	9615.80	156556.30	33998.32	0.0001
TG(58:9)	Triacylglycerol	218515.66	26302.60	52241.90	44062.42	58352.63	10481.51	190860.58	25548.27	289188.96	51524.32	<0.0001
TG(59:3)	Triacylglycerol	96959.22	5312.71	46065.37	10738.08	45343.84	6216.05	78189.52	6458.47	97527.73	17554.98	0.0004
TG(61:8)	Triacylglycerol	65772.64	8682.95	13282.15	18672.56	12768.43	2639.95	68992.21	9304.48	84325.82	16766.74	<0.0001

		Day 7										
Metabolite	**Class**	**Control**	**SEM**	**N_0.25Gy**	**SEM**	**N_1Gy**	**SEM**	**x-ray_1Gy**	**SEM**	**x-ray_4Gy**	**SEM**	**ANOVA p-value**
Linoleic acid	Fatty acid	31636.92	7035.91	20534.33	665.03	23594.15	9060.20	14355.08	1435.20	14849.82	3372.19	0.1445
Docosahexanoic acid	Fatty acid	94345.60	7620.19	75482.58	3502.47	86975.67	16594.89	66071.09	4133.73	66874.04	4819.88	0.1293
Arachidonic acid	Fatty acid	46260.16	4176.12	42143.03	3167.64	43463.55	6379.70	36237.68	4511.89	40907.65	1016.33	0.6407
CE(18:2)	Cholesteryl ester	1687447.60	220106.76	1406673.52	62576.76	1424878.83	78857.67	1793021.10	185012.08	1237049.46	46138.14	0.0994
CE(18:3)	Cholesteryl ester	106800.46	15960.26	88171.98	7988.85	89084.15	4275.57	125150.43	11664.51	72161.42	2544.53	0.0138
CE(20:4)	Cholesteryl ester	2573105.44	271762.78	2342798.73	126248.56	2410951.73	159599.45	3093880.83	216382.47	2065985.85	114540.84	0.0359
CE(20:5)	Cholesteryl ester	408017.66	46314.99	341297.75	23141.60	442959.40	27782.59	490059.97	65823.05	306625.84	19481.51	0.0502
CE(22:6)	Cholesteryl ester	1881823.27	266458.95	1456467.59	84961.99	1448650.74	61719.05	2220982.95	249740.52	1511520.94	101826.14	0.0511
LysoPC(18:0)	Lysophosphatidylcholine	2236752.08	96480.98	1974248.46	138701.31	2052131.15	150303.83	1563354.74	156484.10	1653412.81	126369.91	0.0221
LysoPC(20:1)	Lysophosphatidylcholine	14704.30	1144.19	15859.02	910.59	14689.52	2010.17	11001.71	2539.61	9687.64	1600.58	0.0904
LysoPE(20:0)	Lysophosphatidylethanolamine	30955.81	1300.44	28504.18	2000.28	30235.25	2807.04	24464.36	2573.47	26995.04	3263.03	0.4682
LysoPE(22:0)	Lysophosphatidylethanolamine	20782.83	1060.80	17785.23	1218.79	16036.25	1118.21	13578.15	1836.97	13443.44	1029.69	0.0083
TG(52:1)	Triacylglycerol	52815.01	9231.39	54319.71	3965.75	74306.95	7518.02	83764.99	12153.41	104456.86	6913.69	0.0024
TG(52:3)	Triacylglycerol	1187187.19	165005.04	1281959.80	93410.45	2084986.98	224484.57	1560449.29	181981.55	2103365.32	72037.55	0.0014
TG(55:3)	Triacylglycerol	36257.89	9574.74	42500.16	5417.52	79300.20	10284.49	46697.18	6583.93	62184.46	1367.81	0.0037
TG(56:4)	Triacylglycerol	39860.21	7817.20	47181.89	2378.84	82269.17	9682.71	84409.50	21763.24	145467.99	24896.38	0.0022
TG(56:6)	Triacylglycerol	259420.98	33778.55	276134.37	16759.10	483899.03	41335.88	378187.63	49552.43	541404.80	48798.18	0.0004
TG(56:8)	Triacylglycerol	847178.67	95561.92	839183.89	33307.28	1306647.22	100365.31	1111601.37	128107.71	1374356.75	138036.63	0.0153
TG(57:3)	Triacylglycerol	289023.63	34167.02	317127.83	22981.62	492450.47	49348.13	366112.29	34004.10	482011.33	13521.91	0.0007
TG(57:3)	Triacylglycerol	75402.07	20907.08	62028.90	4814.24	63738.29	4426.45	124908.02	12588.92	77910.45	7354.49	0.0216
TG(57:4)	Triacylglycerol	307537.93	34018.46	316330.63	30111.06	431356.44	30811.86	322944.18	31487.07	395181.16	13652.79	0.0513
TG(58:10)	Triacylglycerol	128638.33	18945.81	130561.31	6670.55	199375.93	11296.45	176902.58	22078.39	245091.04	30904.54	0.0081
TG(58:10)	Triacylglycerol	33709.82	7658.00	34256.94	943.89	74852.84	6734.62	59370.82	10559.77	72304.26	6131.95	0.0023
TG(58:3)	Triacylglycerol	88509.02	13061.04	96518.59	8602.93	159651.50	17462.09	118926.39	12739.01	158369.25	4831.77	0.0009
TG(58:4)	Triacylglycerol	93760.11	12641.95	98859.53	11256.66	146399.66	12438.38	108930.02	14023.09	138307.25	4835.60	0.0282
TG(58:8)	Triacylglycerol	94617.62	12874.04	104864.96	3122.11	184842.52	7719.59	169779.60	20850.41	222271.32	26795.52	0.0003
TG(58:9)	Triacylglycerol	222184.27	31224.53	224954.60	11594.76	386317.51	28910.24	340849.34	42814.44	490939.48	62996.61	0.0012
TG(59:3)	Triacylglycerol	61561.55	9689.99	65222.07	6137.28	101969.30	7465.37	102127.40	13098.80	146017.83	8268.09	<0.0001
TG(61:8)	Triacylglycerol	97363.05	16070.06	90483.98	4616.75	154060.76	14063.73	123857.62	17378.36	152518.42	16710.30	0.0508

Supplementary Table S5: AUC values of each metabolite from individual ROC curves

	Day1 AUC	p-value	Day7 AUC	p-value
		Urine metabolomics		
L-Phenylalanine	1.00	0.0022	0.73	0.28
N-Decanoylglycine	1.00	0.0003	0.73	0.13
Phenylpyruvic acid	0.83	0.04	1.00	0.0003
Sebacic acid	0.72	0.26	0.97	0.003
Xanthurenic acid	0.56	0.93	1.00	0.001
Decanoylcarnitine	0.53	0.86	0.90	0.02
		Serum (metabolomics+lipidomics)		
Linoleic acid	1.00	0.0013	0.57	0.47
Uric acid	1.00	0.0008	0.60	0.47
Eisosapentaenoic acid	1.00	0.0002	0.97	0.02
Linoleic acid_LD	1.00	0.00001	0.60	0.30
Docosahexanoic acid	1.00	0.0004	0.70	0.21
Arachidonic acid_LD	1.00	0.0009	0.70	0.37
LysoPC180	1.00	0.0018	0.83	0.05
LysoPC201	1.00	0.00002	0.67	0.30
LysoPE200	1.00	0.0002	0.73	0.16
LysoPE220	1.00	0.0004	0.70	0.31
Uridine	0.97	0.001	0.57	0.97
L-Carnitine	0.94	0.003	0.83	0.06
Arachidonic acid_pos	0.92	0.014	0.80	0.05
Pyroglutamic acid	0.89	0.025	0.57	0.48
Taurine	0.86	0.047	0.83	0.05
Succinic acid	0.86	0.009	0.57	0.87
Sphinganine-1-phosphate	0.83	0.04	0.87	0.03
L-Tyrosine	0.83	0.03	0.83	0.52
L-Glutamic acid	0.78	0.09	0.67	0.27
Arachidonic acid_neg	0.78	0.13	0.73	0.13
Citric acid	0.64	0.22	0.67	0.42