Analysis of the Urinary Metabolic Profiles in Irradiated Rats treated with Activated Protein C (APC), a Potential Mitigator of Radiation Toxicity

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Untargeted urine metabolomics using UPLC-QToF-MS

(i). Sample preparation: Urine samples were taken out of -80 °C and thawed on ice. To 20 µL of urine sample was added 80 µL of chilled extraction buffer prepared by mixing water:acetonitrile (50:50) and containing internal standards (debrisoquine and 4-nitrobenzoic acid). The samples were vortexed and incubated on ice for 20 minutes followed by incubation at -20 °C for 20 minutes. Finally, the samples were centrifuged at 13000 rpm for 20 minutes at 4 °C. The supernatants were transferred to MS vials for LC-MS data acquisition.

(ii). LC methods and data acquisition: 10 µL from each sample was mixed to generate a pooled quality control (QC) sample. The sample queue was randomized to avoid bias. For metabolomics data acquisition, each sample (1 µL) was injected to a 1.7 µm, 2.1 mm × 50 mm Acquity BEH C18 column (Waters Corporation, MA, USA) using an Acquity UPLC system connected to an electrospray ion source coupled with a quadrupole time-of-flight mass spectrometer (ESI-Q-TOF, Xevo-G2S, Waters Corporation, MA, USA) operating in positive and negative ionization mode. The gradient mobile phases consisted of 100% water with 0.1% formic acid (solvent A), 100% acetonitrile with 0.1% formic acid (solvent B). Each sample injection was run for 11 minutes at a flow rate for 500 µL/min. The LC gradient conditions with a ramp curve of 6 at each step were as follows: Initial – 95% A, 5% B till 0.5 minutes; 4.0 minutes – 80% A, 20% B; 8.0 minutes – 5% A, 95% B till 9.0 minutes; 9.1 minutes – 95% A, 5% B till 11 minutes.

(iii). MS methods: In the MS method, the positive mode had a capillary voltage of 2.5 kV, a sampling cone voltage of 30 V, and a source offset of 80 V. The negative mode had a capillary voltage of 1.0 kV, a sampling cone voltage of 30 V and a source offset of 80 V. The desolvation gas flow was 1000 L/h. and the temperature was set to 500 °C. The cone gas flow was 25 L/h, and the source temperature was 120 °C. The data were acquired in the sensitivity MS Mode with a scan time of 0.3 seconds, and inter-scan delay at 0.014 seconds. The data were acquired in centroid TOF-MS mode over a mass range from 50 to 1,200 m/z. Accurate mass was maintained by infusing Leucine Enkephalin (556.2771 m/z) in 50% aqueous acetonitrile (0.5 ng/mL) at a rate of 20 µL/min via the Lockspray interface for real-time mass correction, every 10 seconds. Before and after samples run, a mixture of six standards (acetaminophen: m/z 152.0712 $[M+H]^+$ / 150.0555 $[M-H]^-$, sulfaguanidine: m/z 215.0603 $[M+H]^+$ / 213.0446 $[M-H]^-$, sulfadimethoxine: m/z 311.0814 $[M+H]^+$ / 309.0658 $[M-H]^-$, Val-Tyr-Val: m/z 380.2185 $[M+H]^+$ / 378.2029 $[M-H]^-$, terfenadine: m/z 472.3216 $[M+H]^+$ and leucine-enkephalin: m/z 556.2771 $[M+H]^+$ / 554.2615 $[M-H]^-$) were run to ensure mass accuracy during data acquisition. Several measures were used to ensure high quality and reproducibility of LC-MS data. The column was conditioned using pooled QC samples, which were injected periodically through the batch to monitor mass accuracy, shifts in retention time and signal intensities as measures of reproducibility. The overlap of QC sample chromatograms (base peak intensity) shows minimal shifts in retention time and consistency in peak intensities throughout the acquisition. Pooled QC samples injected routinely were also used to assess and correct for any analytical variance.

(iv). UPLC-QToF-MS data pre-processing: The MS generated raw data files were first converted into NetCDF files for pre-processing using Waters MassLynx Databridge Software (Waters Corporation). XCMS was used for pre-processing the data files while the Isotopologue Parameter Optimization (IPO) package was used for XCMS parameter optimization.[1] Normalization was performed with internal standards in both positive and negative mode data. The features with more than 20% missing value were also filtered out and the features with less than 20% of missing value were imputed by half of the minimum positive value in the original data. The features with more than 15% of coefficient of variation (CV) were also filtered out. The remaining high-quality features were normalized by QC-RLSC.[2] R package was used to perform multivariate analysis.[3] Statistically significant m/z's with FDR adjusted p-value < 0.05 were run on the UPLC-QToF instrument in the

MS/MS mode. The MS/MS raw data files were converted to NetCDF files using Waters MassLynx Databridge Software, then further converted to MSP file format using an in-house R package. Thereafter, for accurate mass based putative identification of metabolites, we performed database search by matching MS/MS spectra to entries in the NIST 2017 MS/MS database and by applying the online version of CEU Mass Mediator (CMM) which integrated from METLIN, Human Metabolome Database (HMDB) and LIPID MAPS with a ppm error of less than 10.

Targeted urine analysis using 5500 QTRAP

(i). Metabolomics: The targeted metabolomics method was developed in-house to quantitate 270 endogenous molecules using QTRAP® 5500 LC-MS/MS System (Sciex, MA, USA). For the purpose, the sample preparation was kept similar as for untargeted analysis. 5 µL of the prepared sample was injected onto a Kinetex 2.6 µm 100 Å 100 × 2.1 mm (Phenomenex, CA, USA) using SIL-30 AC auto sampler (Shimazdu, Kytoto, Japan) connected with a high flow LC-30AD solvent delivery unit (Shimazdu, Kytoto, Japan) and CBM-20A communication bus module (Shimazdu, Kytoto, Japan) online with QTRAP 5500 (Sciex, MA, USA) operating in positive and negative ion mode. A binary solvent comprising of water with 0.1% formic acid (solvent A) and acetonitrile with 0.1% formic acid (solvent B) was used. The extracted metabolites were resolved at 0.2 mL/min flow rate. The LC gradient conditions were as follows: Initial – 100% A, 0% B for 2.1 minutes; 14 minutes – 5% A, 95% B till 15 minutes; 15.1 minutes – 100% A, 0% B till 22.5 minutes. The auto sampler and oven were kept at 15 °C and 30 °C, respectively. Source and gas setting for the method were as follow: curtain gas = 35, CAD gas = medium, ion spray voltage = 2500 V in positive mode and −4500 V in negative mode, temperature = 400 °C, nebulizing gas = 60 and heater gas = 70.

(ii). Lipidomics: For the purpose, 25 µL of each urine sample was diluted in 125 µL of chilled isopropanol containing internal standards. The samples were vortexed for 1 min and kept on ice for 30 minutes. Samples were incubated at -20 °C for overnight for protein precipitation. The samples were centrifuged at 13,000 rpm for 20 minutes at 4 °C. The supernatant was transferred to MS vial for LC-MS analysis. 10 µL of each prepared sample was mixed to generate the pooled QC sample. 5 µL of the prepared samples were resolved on Xbridge amide 3.5 µm, 4.6 X 100 mm (Waters, MA, USA) column online with a triple quadrupole mass spectrometer (5500 QTRAP, SCIEX, MA, USA) operating in the multiple reaction monitoring (MRM) mode. Each sample was injected using SIL-30 AC auto sampler (Shimazdu, Kyoto, Japan) connected with a high flow LC-30AD solvent delivery unit (Shimazdu, Kyoto, Japan) and CBM-20A communication bus module (Shimazdu, Kyoto, Japan) online with QTRAP 5500 (Sciex, MA, USA) operating in positive and negative ion mode.

Targeted lipidomics method was developed in-house to measure 21 classes of lipid molecules which includes diacylglycerols (DAGs), cholesterol esters (CEs), sphingomyelins (SMs), phosphtatidylchloine (PCs), triacylglycerols (TAGs), free fatty acids (FFAs), ceramides (CERs), dihydroceramides (DCERs), hexosylceramide (HCERs), lactosylceramide (LCERs), phosphatidylethnolamine (PEs), lysophosphtatidylchloine (LPCs), lysophosphatidylethnolamine (LPEs), phosphatidylinositol (PIs), lysophosphatidylinositol (LPIs), phosphatidylserine (PSs), phosphatidic acid (PAs), lysophosphatidic acid (LPAs), monoacyl glycerol (MAGs), acylcarnitines (ACs) and phosphatidyl glycerols (PGs) using QTRAP® 5500 LC-MS/MS System (Sciex, MA, USA). A binary solvent comprising of acetonitrile/water 95/5 with 10 mM ammonium acetate as solvent A and acetonitrile/water 50/50 with 10 mM ammonium acetate as solvent B, was used for the resolution. Lipids were resolved at 0.7 mL/min flow rate. The LC gradient conditions were as follows: Initial – 100% A, 0% B; 3.0 minutes – 99.9% A, 0.1% B; 6.0 minutes – 94% A, 6% B; 10.0 minutes – 75% A, 25% B; 11.0 minutes - 2% A, 98% B, 13.0 minutes – 0% A, 100% B till 18.6 minutes; 18.7 minutes – 100% A, 0% B till 24 minutes. The auto sampler and oven were kept at 15 °C and 35 °C, respectively.

Source and gas setting were as follow: curtain gas = 30, CAD gas = medium, ion spray voltage = 5.5 kV in positive mode and −4.5 kV in negative mode, temperature = 550 °C, nebulizing gas = 50 and heater gas = 60. The reproducibility and high quality of the LC-MS data was ensured using several measures. The column was conditioned using the pooled QC samples initially and pooled QC samples were also injected periodically (after every 10 sample injections) to monitor shifts in signal intensities and retention time as measures of reproducibility and data quality of the LC-MS data. Pooled QC samples were routinely applied to assess and correct for any analytical variance. We also have blank solvent runs between set of samples (after every 10 samples before and after pooled QC samples) to monitor sample-to-sample carry-over effects. To monitor instrumental variance, we also ran NIST plasma sample (every 20 samples) prepared in the same manner as actual samples.

(iii). Data processing and statistical analysis: The abundance measurement for metabolites were expressed as intensity units that were initially normalized to internal standards and processed using MultiQuant 3.0.3 (Sciex). The data were pre-processed using a signal/noise ratio >20:1 and retention time (RT) tolerance of 5 seconds, after manually checking of metabolites peak by experts to find the reliable features. We also use 20% of missing values in each feature as filter out criteria. Missing values were imputed by half of the minimum positive value in the original data. Thereafter, we used 20% of the coefficient of variation (CV) as our filter criteria to remove any possible noises before data normalization. Analytical drifts (if any) were corrected by quality control based robust LOESS signal correction (QC-RLSC). All the analyses were performed in MetaboAnalyst (V5.0) and R (v 4.0.3). The normalized LC-MS data was log transformed and Pareto scaled. For the 183 samples in the study set, the level of differential expression for each metabolite was calculated using an unpaired t-test, comparing sham vs radiation, and radiation vs radiation plus APC treated samples, constrained by FDR corrected *p*-value<0.05. MetaboAnalyst (V5.0) and Mummichog analysis Python package v2.0 was used to evaluate the metabolic pathways affected by radiation exposure longitudinally and radioprotective alleviation by APC treatments. Figures were generated with MetaboAnalyst 5.0, GraphPad Prism 7 (GraphPad Software, La Jolla, CA).

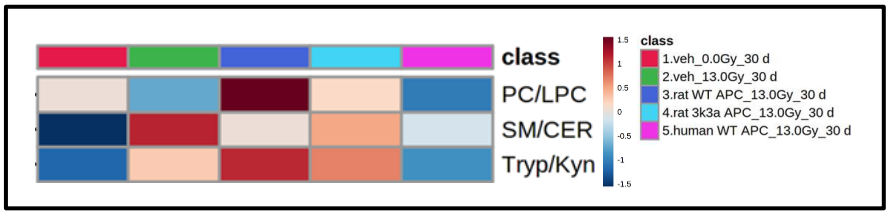


Figure S1. Heatmap showing longitudinal radiation impacts on metabolic ratios for PC/LPC, SM/CER and Trp/Kyn at 30 days post-irradiation.

1. Gowda, H., et al., *Interactive XCMS Online: simplifying advanced metabolomic data processing and subsequent statistical analyses.* Anal Chem, 2014. **86**(14): p. 6931-9.
2. Xia, J., et al., *MetaboAnalyst: a web server for metabolomic data analysis and interpretation.* Nucleic Acids Res, 2009. **37**(Web Server issue): p. W652-60.
3. Dunn, W.B., et al., *Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry.* Nat Protoc, 2011. **6**(7): p. 1060-83.

Supplementary Table 1. List of dysregulated features from global metabolomics profiling of rat urine following exposure to 13.0 Gy of X-ray radiation at 1d, 14d, 30d and 90 d post irradiation and protection by three variants of APC administered at 24h and 48h post irradiation.

		13 Gy vehicle vs. 0 Gy vehicle			
		1d			
m/z_rt	Mode	p.value	FDR	Fold Change	log2(FC)
118.0665_1.68	pos	5.4051E-08	6.5199E-07	0.32218	-1.6341
120.0812_3.26	pos	0.00022808	0.00050841	0.38929	-1.3611
121.0329_0.7	pos	7.3662E-08	7.6012E-07	0.29361	-1.768
121.0661_3.05	pos	9.0559E-09	2.7793E-07	0.26768	-1.9014
123.0452_1.68	pos	7.5382E-07	3.8754E-06	0.41579	-1.2661
124.0405_1.1	pos	8.1231E-08	7.9388E-07	0.31988	-1.6444
126.0928_0.77	pos	4.7939E-07	2.7826E-06	2.4931	1.318
130.0663_4.12	pos	4.3441E-10	9.885E-08	0.15627	-2.6779
133.0534_1.57	pos	0.00010812	0.00025533	0.44419	-1.1708
134.0613_1.57	pos	0.000027487	0.00007463	0.40605	-1.3003
135.0564_1.1	pos	6.3573E-08	7.1473E-07	0.28364	-1.8179
142.0665_3.99	pos	1.6778E-06	9.2024E-06	0.27992	-1.8369
144.046_2.73	pos	0.000058982	0.00014625	0.4333	-1.2066
144.082_1.75	pos	6.6512E-08	7.316E-07	0.11669	-3.0992
144.097_0.31	pos	0.00012501	0.00029624	0.43314	-1.2071
145.0836_1.75	pos	3.3797E-06	0.000012192	0.31548	-1.6644
145.1036_0.33	pos	0.000078927	0.00019021	0.43042	-1.2161
146.0632_1.33	pos	1.4428E-06	0.0000063	0.39508	-1.3398
146.0614_2.6	pos	3.4653E-06	0.000013456	0.32521	-1.6206
146.0946_0.31	pos	4.0581E-06	0.000014332	0.41734	-1.2607
147.0452_3.43	pos	1.618E-06	8.6562E-06	0.27992	-1.8369
152.0637_2.96	pos	1.1641E-05	5.4031E-05	0.21404	-2.2241
158.0318_0.63	pos	5.1218E-10	9.885E-08	0.13296	-2.9109
158.0606_2.94	pos	1.4425E-08	3.5167E-07	0.34096	-1.5523
159.0456_2.45	pos	1.4106E-10	8.0176E-08	0.13066	-2.9361
163.0587_2.05	pos	1.8912E-07	1.3773E-06	0.14855	-2.7509
164.0716_2.61	pos	4.1452E-06	0.000016329	0.33007	-1.5992
164.9974_0.51	pos	0.000007488	0.000023744	0.27166	-1.8801
165.0562_1.16	pos	1.3322E-08	3.3714E-07	0.25751	-1.9573
166.0857_0.57	pos	0.0027903	0.0052539	0.47241	-1.0819
168.1141_1.58	pos	2.5602E-07	1.7747E-06	0.04996	-4.3231
169.0511_1.02	pos	4.6027E-08	5.4738E-07	0.1558	-2.6822
169.0976_0.53	pos	5.6117E-08	6.6649E-07	0.23359	-2.098
170.0611_3.99	pos	2.0007E-06	8.0724E-06	0.2844	-1.814
174.0559_1.26	pos	5.9041E-07	3.2435E-06	0.14694	-2.7667
174.0924_3.19	pos	0.00018827	0.00038573	0.1228	-3.0256
175.1497_2.42	pos	0.00026327	0.00058138	0.35663	-1.4875
176.0718_4.12	pos	4.9456E-10	9.885E-08	0.13863	-2.85
177.0558_2.48	pos	6.1485E-09	2.2603E-07	0.094134	-3.4091
177.0561_1.9	pos	7.7716E-08	7.7202E-07	0.1254	-2.9954
177.1642_4.38	pos	0.000023779	0.000067945	0.16884	-2.5663
180.0562_1.89	pos	4.7563E-06	0.000016271	0.32253	-1.6325
180.1033_5.59	pos	0.000037212	0.000096813	0.32225	-1.6337
180.1089_0.76	pos	6.9222E-08	7.3913E-07	0.1585	-2.6574
181.0617_1.1	pos	1.0791E-07	9.8394E-07	0.31135	-1.6834
181.087_5.41	pos	5.4761E-06	0.000018144	0.40642	-1.299
182.0718_1.09	pos	0.000047482	0.00012176	0.42403	-1.2378
188.1769_0.26	pos	4.9966E-06	6.305E-07	3.7633	1.912
190.0509_1.27	pos	3.4275E-06	0.000012318	0.35138	-1.5007
192.1028_0.56	pos	1.0945E-07	9.8835E-07	0.24485	-2.03
193.0871_2.54	pos	2.735E-08	4.5571E-07	0.17917	-2.4806
197.0803_3.26	pos	1.4929E-07	1.1881E-06	0.36691	-1.4465
197.1187_2.79	pos	4.0678E-08	5.6413E-07	0.15894	-2.6535
203.0441_1.1	pos	1.624E-07	1.2588E-06	0.33092	-1.5954
206.0459_0.92	pos	1.7608E-06	7.3212E-06	0.34719	-1.5262
206.0823_3.4	pos	0.0016098	0.0030313	0.43001	-1.2175
206.1086_0.39	pos	1.9552E-06	7.9164E-06	0.40564	-1.3017
207.1111_0.77	pos	1.1956E-06	5.5049E-06	2.6769	1.4206
209.1183_5.42	pos	6.4022E-07	3.4443E-06	0.15285	-2.7098
212.0915_0.5	pos	1.0936E-08	5.7446E-07	0.31529	-1.6652
221.0821_5.4	pos	3.8335E-06	0.000013432	0.29145	-1.7787
227.0697_4.42	pos	1.2431E-09	1.6604E-07	0.17747	-2.4943
227.084_6.84	pos	0.25306	0.32392	0.82734	-0.27346
228.0516_4.37	pos	1.5805E-08	3.6562E-07	0.097121	-3.3641
231.0777_4.81	pos	0.0000059971	0.000019682	0.15826	-2.6592
232.046_1.21	pos	1.1281E-06	0.000006309	0.25549	-1.9686
484.108_2.29	pos	7.5834E-07	3.8858E-06	0.44846	-1.1571

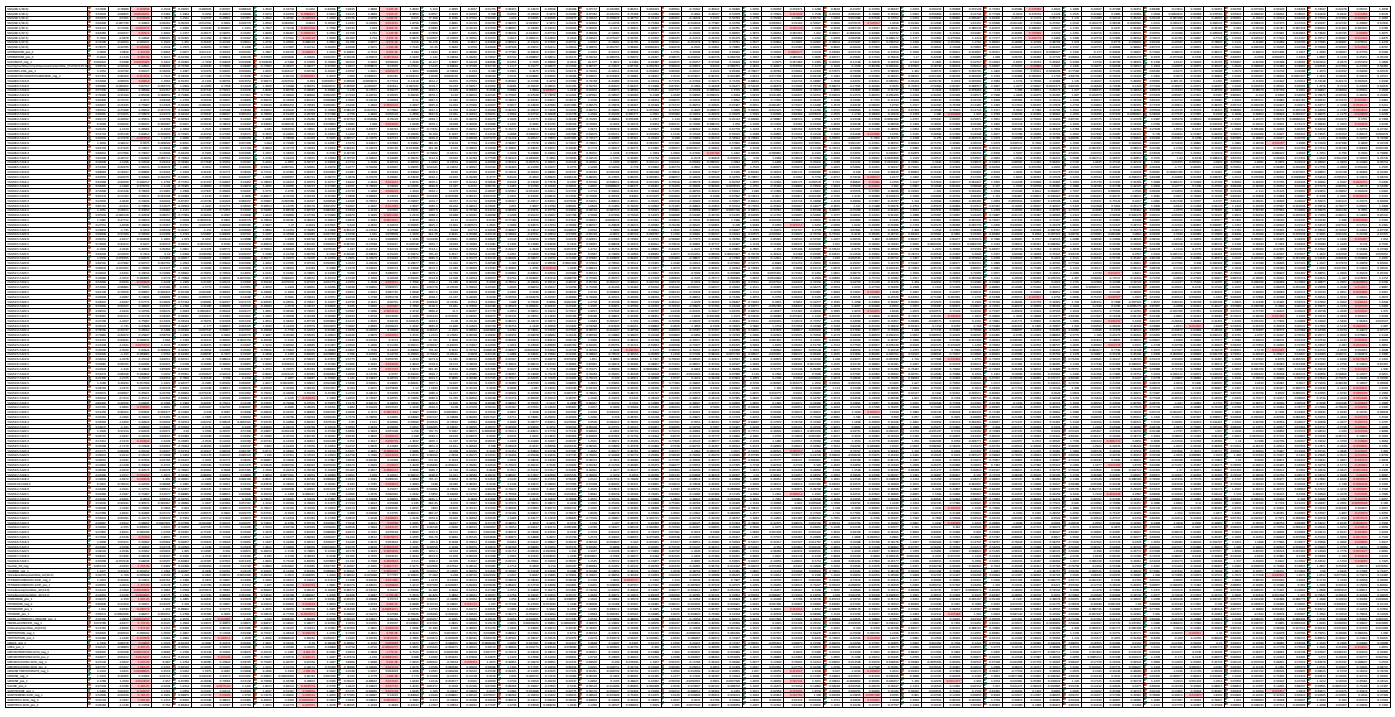
Supplementary Table 2. List of Tandem MS validations for dysregulated metabolites in rat urine following exposure to 13.0 Gy of X-ray radiation at 1d, 14d, 30d and 90 d and potential protection by three APC variants administered at 24h and 48h post irradiation.

Raw data file	precursor_mz_rt	Putative identifications	Synonyms	Adducts	Confidence Level	MSn	CIDs
20210704_medhora_rat_urine_metabolomics_MSMS_POS_11701.CDF	118.0665_1.68	Indole/1H-Indole-3-carboxylic acid		[M+H]+/[M+H-CO2]+	1./1.	MS2/MS2	118.0685,92.0508
20210704_medhora_rat_urine_metabolomics_MSMS_POS_03002.CDF	120.0812_3.26	L-Phenylalanine		[M+H-CH2O2]+	1	MS2	120.0815, 103.0552, 93.0715, 77.0399
20210711_medhora_rat_urine_metabolomics_MSMS_POS_14601.CDF	121.0329_0.7	Shikimic acid/Chorismic acid		[M+H-3H2O]+/[M+H-C3H6O4]+	1./1.	MS2/MS2	121.0474,103.0555,79.0554
20210711_medhora_rat_urine_metabolomics_MSMS_POS_20002.CDF	121.0661_3.05	Tyramine	Phenol, 4-(2-aminoethyl)-	[M+H-NH3]+	2	MS2	121.0659,79.0586
20210704_medhora_rat_urine_metabolomics_MSMS_POS_11801.CDF	123.0452_1.68	Homogentisic acid	Benzeneacetic acid, 2,5-dihydroxy-	[M+H-CH2O2]+	1	MS2	123.0451,105.0340,95.0500,77.0392
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02201.CDF	124.0405_1.1	2,3-Pyridinedicarboxylic acid/Nicotinic acid	Quinolinic acid/3-Pyridinecarboxylic acid	[M+H-CO2]+/[M+H]+	1./2.	MS2/MS2	124.0873, 123.0576, 95.050, 81.0452, 80.0585, 79.0552
20210711_medhora_rat_urine_metabolomics_MSMS_POS_17401.CDF	126.0928_0.77	4,6-Diamino-5-formamidopyrimidine/1-Methylhistamine	FAPy-adenine	[M+H-CO]+/[M+H]+	2./2.	MS2/MS2	126.0656,109.0597
20210711_medhora_rat_urine_metabolomics_MSMS_POS_00803.CDF	130.0663_4.12	1H-Indole-3-propanoic acid/3-Indoleacetic acid		[M+H-C2H4O2]+/[M+H-CH2O2]+	2./2.	MS2/MS2	130.0660,103.0554
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09001.CDF	133.0534_1.57	D-Asparagine	D-2,4-Diamino-4-oxobutanoic acid	[M+H]+	1	MS2	133.0539,105.0371,91.0555,79.0559
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09101.CDF	134.0613_1.57	DL-Normetanephrine/5-Hydroxyindole		[M+H-CH6O2]+/[M+H]+	1./1.	MS2/MS2	134.0611,117.0692,106.0660,96.0455
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02301.CDF	135.0564_1.1	DL-3,4-Dihydroxyphenyl glycol/Cresotinic acid	1,2-Benzenediol, 4-(1,2-dihydroxyethyl)-/2-Hydroxy-3-methylbenzoic acid	[M+H-2H2O]+/[M+H-H2O]+	2./2.	MS2/MS2	135.0575,120.0456,105.0352
20210704_medhora_rat_urine_metabolomics_MSMS_POS_14302.CDF	142.0665_3.99	N-Isovalerylglycine	Glycine, N-(3-methyl-1-oxobutyl)-	[M+H-H2O]+	2	MS2	142.0668,115.0555
20210711_medhora_rat_urine_metabolomics_MSMS_POS_13202.CDF	144.046_2.73	Kynurenic acid		[M+H-CH2O2]+	1	MS2	144.0605, 129.0350, 119.0504, 101.0389
20210704_medhora_rat_urine_metabolomics_MSMS_POS_13101.CDF	144.082_1.75	N-Methyltryptamine	1H-Indole-3-ethanamine, N-methyl-	[M+H-CH5N]+	1	MS2	146.0612,145.0840,144.0816,128.0506,119.0508
20210711_medhora_rat_urine_metabolomics_MSMS_POS_02101.CDF	144.097_0.31	L-Homoarginine/3-(2-Hydroxyethyl)indole	L-Lysine, N6-(aminoiminomethyl)-/Tryptophol	[M+H-CH3ON]+/[M+H-H2O]+	2./1.	MS2/MS2	144.1002,84.0806
20210704_medhora_rat_urine_metabolomics_MSMS_POS_13201.CDF	145.0836_1.75	DL-5-Hydroxylysine		[M+H-H2O]+	2	MS2	145.0830,128.0502
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02201.CDF	145.1036_0.31	DL-5-Hydroxylysine		[M+H-H2O]+	2	MS2	145.1035,128.0504,84.0811
20210704_medhora_rat_urine_metabolomics_MSMS_POS_06801.CDF	146.0612_1.33	5-Hydroxyindole-3-acetic acid	1H-Indole-3-acetic acid, 5-hydroxy-	[M+H-CH2O2]+	2	MS2	146.0613,128.0507,119.0513
20210711_medhora_rat_urine_metabolomics_MSMS_POS_09202.CDF	146.0614_2.6	5-Hydroxyindole-3-acetic acid	1H-Indole-3-acetic acid, 5-hydroxy-	[M+H-CH2O2]+	1	MS2	146.0613,128.0501,119.0517,101.0398,77.0399
20210711_medhora_rat_urine_metabolomics_MSMS_POS_02301.CDF	146.0946_0.31	N-Isobutyrylglycine	Glycine, N-(2-methyl-1-oxopropyl)-	[M+H]+	2	MS2	146.0608,128.0496
20210704_medhora_rat_urine_metabolomics_MSMS_POS_05602.CDF	147.0452_3.43	2-Methylglutaric acid/Adipic acid	Pentanedioic acid, 2-methyl-/Hexanedioic acid	[M+H]+/[M+H]+	1./1.	MS2/MS2	147.0455,129.0347,103.0552,101.0395
20210711_medhora_rat_urine_metabolomics_MSMS_POS_17302.CDF	152.0637_2.96	Pyridoxine	Vitamin B6	[M+H-H2O]+	2	MS2	152.0628,137.0255
20210711_medhora_rat_urine_metabolomics_MSMS_POS_11901.CDF	158.0318_0.63	S-Methyl-L-cysteine	(R)-2-Amino-3-(methylmercapto)propionic acid	[M+Na]+	2	MS2	158.0692,113.0351
20210711_medhora_rat_urine_metabolomics_MSMS_POS_15902.CDF	158.0606_2.94	Indole-3-pyruvic acid/Guanidinosuccinic acid	/L-Aspartic acid, N-(aminoiminomethyl)-	[M+H-CH2O2]+/[M+H-H2O]+	1./2.	MS2/MS2	158.0655,130.0656,103.0549
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_22401.CDF	158.0819_1.47	N-Acetyl-DL-valine		[M-H]-	2	MS2	158.0816,114.0918
20210711_medhora_rat_urine_metabolomics_MSMS_POS_06102.CDF	159.0456_2.45	L-Dihydroorotic acid/Ureidosuccinic acid	/DL-2-Ureidobutanedioic acid	[M+H]+/[M+H-H2O]+	1./1.	MS2/MS2	159.0814,131.0510,116.0500,89.0392
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_28601.CDF	159.0658_1.88	3-Methyladipic acid/2,2-Dimethylglutaric acid	3-Methylhexanedioic acid	[M-H]-	1	MS2	159.0555,14.0536,115.0754,97.0656,95.0502
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01102.CDF	163.0587_2.05	Chorismic acid		[M+H-CH4O3]+	1	MS2	163.0588, 162.0560, 145.0480, 144.0453, 118.0658, 105.0349, 95.0505, 91.0548, 89.0397, 79.0554, 77.0393
20210711_medhora_rat_urine_metabolomics_MSMS_POS_09802.CDF	164.0716_2.61	L-Carnosine/4-Hydroxy-L-glutamic acid	β-Alanyl-L-histidine	[M+H-CH5O2N]+/[M+H]+	1./2.	MS2/MS2	164.0712,147.0459,136.0752,119.0519,107.0832
20210711_medhora_rat_urine_metabolomics_MSMS_POS_07901.CDF	164.9974_0.51	Benzoyl coenzyme A	Coenzyme A, S-benzoate	[M+2H]2+	2	MS4	165.0603,146.0603,120.0816
20210704_medhora_rat_urine_metabolomics_MSMS_POS_03401.CDF	165.0562_1.16	p-Hydroxyphenyllactic acid/L-Tyrosine		[M+H-H2O]+/[M+H-NH3]+	1./1.	MS2/MS2	165.0596,137.0606,12.0807,109.0714,77.0393
20210711_medhora_rat_urine_metabolomics_MSMS_POS_10601.CDF	166.0857_0.57	L-Phenylalanine/(-)-Epinephrine	/(-)-Adrenaline	[M+H]+/[M+H-H2O]+	1./1.	MS2/MS2	166.0741,149.0466,120.0812
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09401.CDF	168.1141_1.58	Suberylglycine/3-Methoxytyramine	Octanoic acid, 8-[(carboxymethyl)amino]-8-oxo-/3-O-Methyldopamine	[M+H-CH4O3]+/[M+H]+	1./1.	MS2/MS2	168.1135,152.0343,138.0611,122.0656,98.0917
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01101.CDF	169.0511_1.02	Uric acid	2,6,8-Trihydroxypurine	[M+H]+	2	MS2	169.0908,152.0350,126.0673,109.0770,95.0252,83.0418,68.9875
20210711_medhora_rat_urine_metabolomics_MSMS_POS_09501.CDF	169.0976_0.53	Pyridoxamine/L-Lysine	/(S)-2,6-Diaminohexanoic acid	[M+H]+/[M+Na]+	1./1.	MS2/MS2	169.1023,152.0342,124.0854,109.0758,96.0697
20210704_medhora_rat_urine_metabolomics_MSMS_POS_14402.CDF	170.0611_3.99	DL-Indole-3-lactic acid/3-Indoleacrylic acid		[M+H-2H2O]+/[M+H-H2O]+	1./1.	MS2/MS2	170.0611,142.0661,115.0467
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_04902.CDF	171.0657_2.3	L-Homocitrulline/DL-α-Lipoic acid	L-Lysine, N6-(aminocarbonyl)-/2,6-Diaminoheptanedioic acid	[M-H-NH3]-/[M-H-H2S]-	1./1.	MS2/MS2	153.0924,128.0720,127.0765,111.0816,83.0499
20210704_medhora_rat_urine_metabolomics_MSMS_POS_05301.CDF	174.0559_1.26	Orotic acid	6-Carboxyuracil	[M+NH4]+	1	MS2	174.1289,159.0926,146.0624,142.0661,128.0577,115.0543,87.0443
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02402.CDF	174.0924_3.19	Melatonin	Acetamide, N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-	[M+H-C2H5ON]+	1	MS2	174.0854,158.0921,130.0661,117.0323,103.0555
20210711_medhora_rat_urine_metabolomics_MSMS_POS_05802.CDF	175.1497_2.42	5α-Androstane-3α,17β-diol		[M+H-C6H14O2]+	1	MS2	175.0948,145.0295,131.0658,119.0760,105.0707,91.0553
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01103.CDF	176.0718_4.12	3-Indoleacetic acid/Guanidinosuccinic acid	/L-Aspartic acid, N-(aminoiminomethyl)-	[M+H]+/[M+H]+	2./2	MS2/MS2	176.0769,151.0709,130.0661,103.0556,105.0712
20210711_medhora_rat_urine_metabolomics_MSMS_POS_06502.CDF	177.0558_2.48	Allantoic acid/Ureidosuccinic acid	Acetic acid, diureido-/Aspartic acid, N-(aminocarbonyl)-	[M+H]+/[M+H]+	1./1.	MS2/MS2	177.1140,160.0760,145.0297,134.0970,117.0606
20210704_medhora_rat_urine_metabolomics_MSMS_POS_14501.CDF	177.0561_1.9	Allantoic acid/Ureidosuccinic acid	Acetic acid, diureido-/Aspartic acid, N-(aminocarbonyl)-	[M+H]+/[M+H]+	2./1.	MS2/MS2	177.1148,134.0970,117.0599,91.0548
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03703.CDF	177.1642_4.38	Tetradecanedioic acid	1,12-Dodecanedicarboxylic acid	[M+H-CH6O4]+	1	MS2	177.1644,103.0543
20210704_medhora_rat_urine_metabolomics_MSMS_POS_13801.CDF	180.0562_1.89	Hippuric acid	Glycine, N-benzoyl-	[M+H]+	1	MS2	180.0670,105.0344,95.0499,77.0391
20210704_medhora_rat_urine_metabolomics_MSMS_POS_04403.CDF	180.1033_5.59	Metanephrine/Tetrahydro-L-biopterin	4-Hydroxy-3-methoxy-N-methylphenethanolamine	[M+H-H2O]+/[M+H-H2O]+	1./2	MS2/MS3	180.1017,151.0908,136.0859,120.0816,105.0712,91.0512,79.0557
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16501.CDF	180.1039_0.76	Metanephrine	4-Hydroxy-3-methoxy-N-methylphenethanolamine	[M+H-H2O]+	1	MS2	180.0970,136.0636,124.0405,106.0299,96.0455
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02501.CDF	181.0617_1.1	4-Hydroxyphenylpyruvic acid/Nitrotyrosine	Benzenepropanoic acid, 4-hydroxy-α-oxo-/	[M+H]+/[M+H-CH2O2]+	1./1.	MS2/MS2	163.0532, 153.0598, 137.0704, 135.0570, 123.0806, 77.0394
20210711_medhora_rat_urine_metabolomics_MSMS_POS_00803.CDF	181.087_5.41	1,11-Undecanedicarboxylic acid/Prostaglandin I2	Brassylic acid	[M+H-H2O]+/[M+H]+	2./2.	MS3/MS3	181.0920, 135.0819, 123.0820, 121.0707
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02001.CDF	182.0718_1.09	L-Tyrosine/N-Isovalerylglycine	/Glycine, N-(3-methyl-1-oxobutyl)-	[M+H]+/[M+Na]+	1./1.	MS2/MS2	182.0875,165.0942,136.0616,123.0787
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01001.CDF	188.1769_0.26	N8-Acetylspermidine	Acetamide, N-[4-[(3-aminopropyl)amino]butyl]-	[M+H]+	1	MS2	188.0764,163.0591,115.0544,84.0820
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_07402.CDF	190.0505_2.59	5-Hydroxyindole-3-acetic acid/L-Kynurenine	/Benzenebutanoic acid, α,2-diamino-γ-oxo-, (S)-	[M-H]-/[M-H-NH3]-	1./1.	MS2/MS2	190.0509,146.0612,144.0456,133.0298,131.0376
20210704_medhora_rat_urine_metabolomics_MSMS_POS_05501.CDF	190.0509_1.27	Kynurenic acid	2-Quinolinecarboxylic acid, 4-hydroxy-	[M+H]+	1	MS2	190.0512,162.0564,144.0461,116.0507,89.0391
20210711_medhora_rat_urine_metabolomics_MSMS_POS_10201.CDF	192.1032_0.56	5-Methoxytryptophol	1H-Indole-3-ethanol, 5-methoxy-	[M+H]+	1	MS2	192.1032,146.0605,128.0205,117.0477
20210711_medhora_rat_urine_metabolomics_MSMS_POS_07202.CDF	193.0871_2.54	Sinapyl alcohol	p-Hydroxy-m,m'-dimethoxycinnamyl alcohol	[M+H-H2O]+	2	MS2	193.0935,146.0624,92.0584,91.0552
20210704_medhora_rat_urine_metabolomics_MSMS_POS_03202.CDF	197.0803_3.26	N-α-Acetyl-L-ornithine		[M+Na]+	2	MS2	197.0724, 179.1041, 169.0692, 153.0713, 152.0679, 123.0487
20210711_medhora_rat_urine_metabolomics_MSMS_POS_14002.CDF	197.1187_2.79	L-Arginine/Estrone		[M+Na]+/[M+H-H2O]+	1./1.	MS2/MS3	197.0701,179.1028,169.0669,141.0662
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02701.CDF	203.0441_1.1	Nicotinuric acid	Glycine, N-(3-pyridinylcarbonyl)-	[M+Na]+	2	MS2	203.1588, 202.0529, 188.0543, 160.0410, 158.1176, 157.0771, 145.0427, 143.1075, 111.0462, 100.0771, 85.0275,
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20402.CDF	204.0661_3.39	DL-Indole-3-lactic acid	1H-Indole-3-propanoic acid, α-hydroxy-	[M-H]-	1	MS2	204.0662,186.0558,158.0606,142.0660,128.0495,116.0506,72.9978
20210704_medhora_rat_urine_metabolomics_MSMS_POS_20301.CDF	206.0459_0.92	Xanthurenic acid/4-Pyridoxic acid	8-Hydroxykynurenic acid	[M+H]+/[M+Na]+	1./1.	MS2/MS2	206.0464,188.0545,178.0506,160.0413,132.0450
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19702.CDF	206.0817_3.26	N-Acetyl-L-phenylalanine		[M-H]-	1	MS2	206.0807,164.0690,147.0451,91.0540
20210704_medhora_rat_urine_metabolomics_MSMS_POS_05102.CDF	206.0823_3.4	DL-Indole-3-lactic acid	1H-Indole-3-propanoic acid, α-hydroxy-	[M+H]+	1	MS2	206.0835,188.0721,170.0618,160.0760,146.0598,130.0665,118.0658
20210711_medhora_rat_urine_metabolomics_MSMS_POS_05801.CDF	206.1086_0.39	Tetrahydro-L-biopterin		[M+H-2H2O]+	2	MS2	See 203A
20210711_medhora_rat_urine_metabolomics_MSMS_POS_17701.CDF	207.1111_0.77	7α-Hydroxyandrostenedione	Androst-4-ene-3,17-dione, 7-hydroxy-, (7α)-	[M+H]+	2	MS4	207.0908,192.1022,191.1050,179.0562,178.0503
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01403.CDF	209.1183_5.42	rac-all-trans-4-Hydroxyretinal		[M+H-C6H12O2]+	1	MS2	209.1180,194.1086,179.0860,165.0744,149.0967,117.0690
20210711_medhora_rat_urine_metabolomics_MSMS_POS_07801.CDF	212.0915_0.5	L-Homocitrulline/D-Glucuronic acid	L-Lysine, N6-(aminocarbonyl)-/Glucosiduronic acid	[M+Na]+/[M+NH4]+	2./2.	MS2/MS2	212.1036,194.0899,169.0672,96.0694,84.0816,
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_12001.CDF	215.997_0.69	4-Thiouridine	Uridine, 4-thio-	[M-H]-	2	MS3	215.9975,158.0805,125.08773,120.0219,98.9881,92.0270
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_09801.CDF	218.1028_0.64	Pantothenic acid	β-Alanine, N-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-	[M-H]-	1	MS2	218.0576,146.0818,88.0403,71.0495
20210711_medhora_rat_urine_metabolomics_MSMS_POS_21003.CDF	221.0821_5.4	5-Hydroxy-L-tryptophan/Indole-3-pyruvic acid	Oxitriptan	[M+H]+/[M+NH4]+	1./1.	MS2/MS2	221.0915,175.0828,162.0714,134.0756
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_08003.CDF	223.095_5.32	Prostaglandin K2	9,11-Dioxo-15S-hydroxy-5Z,13E-prostadienoic acid	[M-H]-	2	MS3	223.0828,177.0900,163.1127,151.1018,137.0959
20210711_medhora_rat_urine_metabolomics_MSMS_POS_04603.CDF	227.0697_4.42	Biotin/5-Acetylamino-6-formylamino-3-methyluracil		[M+H-H2O]+/[M+H]+	1./2	MS2/MS2	227.0750,209.1178,199.0752,182.0533,163.0888,143.0468,123.0828,115.0558
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03904.CDF	227.084_6.84	Retinyl acetate/Trihydroxycoprostane		[M+H-C2H4O2]+/[M+H-3H2O]+	1./1.	MS3/MS3	227.1643,169.1035,157.0923,145.0997
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03303.CDF	228.0516_4.37	DL-Indole-3-lactic acid	1H-Indole-3-propanoic acid, α-hydroxy-	[M+Na]+	2	MS2	228.0489,182.0586
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_15403.CDF	229.1444_6	Dodecanedioic acid	1,10-Decanedicarboxylic acid	[M-H]-	1	MS2	229.1420,211.1263,167.1438,71.0489
20210711_medhora_rat_urine_metabolomics_MSMS_POS_14703.CDF	231.0777_4.81	3-Methylglutarylcarnitine		[M+H-C3H9N]+	1	MS2	231.0798,185.0726,147.0642
20210704_medhora_rat_urine_metabolomics_MSMS_POS_03801.CDF	232.046_1.21	Pyridoxamine 5-phosphate		[M+H-NH3]+	2	MS2	232.1535,122.0350,107.0482,91.0552
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16401.CDF	232.1554_0.75	Isobutyryl-L-carnitine		[M+H]+	1	MS2	232.1537,173.0849,85.0249
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16102.CDF	233.0952_2.94	5-trans-Prostaglandin D2/Coenzyme Q1	Ubiquinone-1	[M+H-2H2O]+/[M+H]+	2./2.	MS3/MS3	233.0947,187.0892,147.0902,131.0691,91.0554
20210711_medhora_rat_urine_metabolomics_MSMS_POS_14902.CDF	235.0823_2.92	13,14-Dihydro-15-ketotetranorprostaglandin D2/13-Hydroperoxy-9Z,11E-	/13-HpODE	[M+H-2H2O]+/[M+Na]+	1./1.	MS3/MS3	235.1128,217.0995,191.0835,147.0907,133.0705,91.0547
20210704_medhora_rat_urine_metabolomics_MSMS_POS_04903.CDF	237.1179_5.7	N-α-Acetyl-N-2-formyl-5-methoxykynurenamine		[M+H-CO]+	1	MS2	237.0790,145.0976,134.0976,121.0657
20210711_medhora_rat_urine_metabolomics_MSMS_POS_12002.CDF	237.1219_2.7	N-α-Acetyl-N-2-formyl-5-methoxykynurenamine		[M+H-CO]+	2	MS2	237.0587,134.0962,130.0654,121.0671
20210711_medhora_rat_urine_metabolomics_MSMS_POS_06301.CDF	239.1014_0.41	16α-Hydroxy-4-androstene-3,17-dione/Cholesta-4,6-dien-3-one		[M+H-2H2O]+/[M+H-H2O]+	1./2.	MS3/MS3	239.1014,224.0862,196.0967,181.0657,168.0984,
20210704_medhora_rat_urine_metabolomics_MSMS_POS_15902.CDF	239.1398_3.96	4-Androsten-11β-ol-3,17-dione/N-Acetyl-D-glucosamine		[M+H-C2H8O2]+/[M+NH4]+	1./2.	MS2/MS2	239.1379,197.1291,133.0649,117.0703,105.0708,79.0557
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01703.CDF	239.1662_5.44	5α-Pregnan-17-ol-3,20-dione		[M+H-C3H10O3]+	1	MS2	239.1789,224.1774,181.0868,145.0932,121.0683,91.0551
20210711_medhora_rat_urine_metabolomics_MSMS_POS_07403.CDF	242.0955_4.46	α-D-Galactosamine 1-phosphate/11-Dehydrocorticosterone		[M+H]+/[M+H]+	2./1.	MS3/MS4	242.1767,227.0712,199.0777,182.0880,170.0606,121.0646
20210711_medhora_rat_urine_metabolomics_MSMS_POS_12301.CDF	242.101_0.64	Pantothenic acid/α-D-Galactosamine 1-phosphate		[M+Na]+/[M+H]+	1./1.	MS3/MS3	242.1341,224.0858,214.1151,196.0967,168.1017,112.0778
20210711_medhora_rat_urine_metabolomics_MSMS_POS_12401.CDF	243.135_0.64	all-trans-4-Hydroxyretinoic acid	Retinoic acid, 4-hydroxy-	[M+H-C4H10O]+	2	MS2	243.1343,225.1310,215.1242,201.0773,181.0990,163.0574,156.0966
20210704_medhora_rat_urine_metabolomics_MSMS_POS_14101.CDF	246.1714_1.89	Isovaleryl-L-carnitine		[M+H]+	1	MS2	246.1701,187.0979,85.0297
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03403.CDF	247.0031_4.37	D-α-Tocopherol succinate		[M+H-C23H38]+	1	MS3	247.0048,227.0454,177.0730,162.0878,134.0932,107.0529
20210711_medhora_rat_urine_metabolomics_MSMS_POS_21103.CDF	249.1115_5.4	15S-Hydroperoxy-11Z,13E-eicosadienoic acid	15(S)-HpEDE	[M+H-H2O]+	2	MS4	249.1132,193.0904,149.0967
20210711_medhora_rat_urine_metabolomics_MSMS_POS_04102.CDF	252.0888_2.29	4-Androsten-11β-ol-3,17-dione	11β-Hydroxyandrostenedione	[M+H-H2O]+	2	MS4	252.1612,237.0550,209.0611,197.0601,181.0651,171.0800
20210711_medhora_rat_urine_metabolomics_MSMS_POS_11503.CDF	253.1449_4.56	Estriol	16α-Hydroxyestradiol	[M+H-2H2O]+	1	MS2	253.0584,207.1350,193.1213,181.0652,153.0701,115.0546,91.0551
20210711_medhora_rat_urine_metabolomics_MSMS_POS_06401.CDF	254.1121_0.41	Suberylglycine/N-Glycolylneuraminic acid		[M+Na]+/[M+H-3H2O]+	2./2.	MS2/MS3	254.1161,237.0898,210.1153,197.1216,166.0978
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_03701.CDF	254.9813_0.33	Uridine 5'-diphosphoglucuronic acid		[M-H]-	2	MS3	254.9812,210.9511,175.0242,115.0036,111.0105,96.9603
20210704_medhora_rat_urine_metabolomics_MSMS_POS_07702.CDF	257.0828_3.69	L-Thyronine	L-Tyrosine, O-(4-hydroxyphenyl)-	[M+H-NH3]+	1	MS2	257.0846,210.0668,181.0661,164.0523,152.0636,128.0598,123.0454,116.0707,107.0507,95.0513
20210704_medhora_rat_urine_metabolomics_MSMS_POS_07001.CDF	259.2031_1.37	Tetradecanedioic acid/19-Norandrosterone	/Estran-17-one, 3-hydroxy-, (3α,5α)-	[M+H]+/[M+H-H2O]+	1./1.	MS2/MS2	259.1804,241.1522,197.1177,175.0871
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_14101.CDF	261.0071_0.84	Homovanillic acid sulfate	Benzeneacetic acid, 3-methoxy-4-(sulfooxy)-	[M-H]-	1	MS2	261.0072,217.0490,179.0346,166.0273,153.0551,137.0806,122.0368
20210711_medhora_rat_urine_metabolomics_MSMS_POS_15703.CDF	261.1144_4.95	Monolinolenin (9c,12c,15c)/18-Carboxydinorleukotriene B4	1-Linolenoylglycerol	[M+H-H2O]+/[M+H-H2O]+	1./2	MS3/MS4	261.1229,243.1062,199.0752,175.0798,135.0808,113.0595,91.0548
20210711_medhora_rat_urine_metabolomics_MSMS_POS_05201.CDF	261.1151_0.36	Monolinolenin (9c,12c,15c)/β-Hyodeoxycholic acid	1-Linolenoylglycerol	[M+H-H2O]+/[M+H-3H2O]+	2./2.	MS3/MS3	See 157C
20210704_medhora_rat_urine_metabolomics_MSMS_POS_00903.CDF	263.0907_5.41	all-trans-5,6-Epoxyretinoic acid/Mannotriose	18:0-18:2 DAG/Glycan Mannotriose	[M+H-2H2O]+/[M+H+K]2+	1./1.	MS3/MS3	263.0997, 248.0929, 247.1194, 245.1028, 231.0901, 219.1197, 217.1123, 205.1104, 167.1010, 139.0699
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_29201.CDF	263.1047_1.92	Phenylacetyl-L-glutamine		[M-H]-	1	MS2	263.0237,145.0613,127.0507,125.0250,81.9828,74.0239
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16503.CDF	263.1103_5.13	all-trans-5,6-Epoxyretinoic acid		[M+H-2H2O]+	1	MS3	263.0999,245.1060,222.0001,173.0731,133.0660,91.0557
20210711_medhora_rat_urine_metabolomics_MSMS_POS_04201.CDF	267.1351_0.34	6-Ketoestriol	6-Oxo-16α,17β-estriol	[M+H-2H2O]+	2	MS2	267.1349,229.1220,192.9942,183.1150,166.0964,154.0803,139.0477,107.0513
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02303.CDF	267.1966_5.5	13-cis-Retinal	13-cis-Retinaldehyde	[M+H-H2O]+	1	MS3	267.1795, 225.1147, 197.0663, 187.0768, 183.0781, 169.0695, 159.0556, 155.0631, 145.0393, 135.0413, 133.1021, 131.0613, 121.0413, 119.0584, 91.0550, 69.0125
20210711_medhora_rat_urine_metabolomics_MSMS_POS_09701.CDF	269.0911_0.53	7α-Hydroxydehydroepiandrosterone/15(R),19(R)-Hydroxyprostaglandin E2	7α-Hydroxy-DHEA	[M+H-H2O]+/[M+H-H2O]+	1./2.	MS3/MS4	268.9488,225.1238,211.0927,183.1142,141.0645,123.0568,107.0512
20210711_medhora_rat_urine_metabolomics_MSMS_POS_12303.CDF	273.1138_4.68	Argininosuccinic acid		[M+H]+	2	MS3	273.0884,256.2028,228.0491,209.9994,150.0238,130.0671
20210711_medhora_rat_urine_metabolomics_MSMS_POS_02501.CDF	273.1158_0.31	8-iso-15-Ketoprostaglandin F2α/Cholest-5-ene-3b,20,22R-triol	/Oxy-16	[M+H]+/[M+H-H2O]+	2./2.	MS4/MS3	273.1800,227.1372,185.1190,169.0925
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09403.CDF	273.222_6.25	5α-Androsterone	17α-Hydroxy-5α-pregnane-3,20-dione	[M+H-H2O]+	2	MS3	273.2114,155.0562,142.0761,106.0869,91.0547,70.0655
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_23801.CDF	275.0228_1.63	6-Phosphogluconic acid	D-Gluconic acid, 6-(dihydrogen phosphate)	[M-H]-	2	MS2	275.0210,177.0545,129.0375,96.9600
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02801.CDF	275.0911_1.13	8-Hyodeoxycholic acid/21-Deoxycortisol	Cholan-24-oic acid, 3,6-dihydroxy-, (3β,5β,6α)-/11β,17α-Dihydroxyprogesterone	[M+H-2H2O]+/[M+H-3H2O]+	1./1.	MS3/MS3	275.1108, 257.1569, 232.9840, 207.0014, 205.9937, 192.0097, 197.0049, 169.1010, 158.9401, 154.9997, 145.0272, 129.0934
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01401.CDF	277.1084_1.04	13-Hydroperoxy-9Z,11E-octadecadienoic acid/4-Pregnen-6β,11β,17,21-tetrol-3,20-	13-HpODE/6β-Hydroxycortisol	[M+Na]+/[M+H-CH8O4]+	1./1.	MS3/MS3	277.1173,189.0975,175.1182,123.0773
20210711_medhora_rat_urine_metabolomics_MSMS_POS_10203.CDF	281.1188_4.49	20-Carboxyarachidonic acid/15-Hydroperoxy-5Z,8Z,11Z,13E,17Z-eicosapentaenoic acid	5Z,8Z,11Z,14Z-Eicosatetraenedioic acid/15-HpEPE	[M+H-H2O]+/[M+H-2H2O]+	2./1.	MS3/MS3	281.1229,263.1100,235.1107,187.0761,161.0672,131.0657,105.0705
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16603.CDF	282.1233_5.13	N-Acetyl[illegible]/Protoporphyrin IX		[M+H-3H2O]+/[M+2H]2+	2./2.	MS2/MS2	282.1226,264.1221,247.0882,196.0637,168.0613,149.0621,133.0657,107.0570
20210704_medhora_rat_urine_metabolomics_MSMS_POS_14602.CDF	283.0493_3.99	Cinnabarinic acid		[M+H-H2O]+	1	MS2	283.1191,242.0539,229.0855,224.0348,213.0533,200.0771,194.9859,185.0484,167.0351,155.0189,141.0691,129.0670,118.0431
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01302.CDF	283.1149_3.15	9-Hydroxy-5Z,7E,11Z,14Z,17Z-eicosapentaenoic acid/5β-Pregnane-3α,17,21-triol-11,20	(±)9-HEPE/5β-Tetrahydrocortisone	[M+H-H2O]+/[M+H-3H2O]+	1./1.	MS3/MS3	283.1183,265.1150,241.0627,213.0554,194.9961,167.0363,141.0701,109.0366,
20210704_medhora_rat_urine_metabolomics_MSMS_POS_00802.CDF	284.1055_3.12	8-Hydroxy-2'-deoxyguanosine/Guanosine	Guanosine, 2'-deoxy-7,8-dihydro-8-oxo-/Guanine-9-β-D-ribofuranoside	[M+H]+/[M+H]+	1./2.	MS2/MS2	284.1107,283.1189,169.0664,168.0579
20210711_medhora_rat_urine_metabolomics_MSMS_POS_07503.CDF	285.1119_4.46	N-(2-Hydroxyethyl)-5(6)-epoxy-8Z,11Z,14Z-eicosatrienamide/4-Methoxy-17β-estradiol	5(6)-EET ethanolamide/	[M+H-H2O]+/[M+H]+	1./1.	MS3/MS3	285.0766,257.0818,229.1016,197.0619,169.0690,141.0716,107.0536,
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03504.CDF	285.1877_6.55	19-Hydroxyandrost-4-ene-3,17-dione/1,25-Dihydroxy Vitamin D2		[M+H-H2O]+/[M+H-C9H20O]+	1./1.	MS2/MS2	285.1647,241.1563,215.1191,131.0863
20210704_medhora_rat_urine_metabolomics_MSMS_POS_10902.CDF	286.2026_3.84	Prostaglandin B3	PGB3	[M+Na]+	2	MS3	286.0850,271.0575,257.0868,243.0666,229.0851,214.0638,203.9891,186.0616,169.0642
20210711_medhora_rat_urine_metabolomics_MSMS_POS_15003.CDF	286.2029_4.92	Prostaglandin B3		[M+Na]+	2	MS3	286.1614,271.0693,257.0895,243.0749,229.1097,213.0682,186.0822,169.0672
20210711_medhora_rat_urine_metabolomics_MSMS_POS_18503.CDF	288.2179_5.2	Octanoylcarnitine		[M+H]+	2	MS2	288.2102,85.0292
20210711_medhora_rat_urine_metabolomics_MSMS_POS_10903.CDF	291.1208_4.53	9(11)-Dehydroestriol		[M+Na-H2O]+	2	MS2	291.1214,229.0820,122.0975
20210711_medhora_rat_urine_metabolomics_MSMS_POS_21001.CDF	295.0941_0.97	Monoarachidin/3α,21-Dihydroxy-5β-pregnane-11,20-dione	Monoeicosenoin (MAG)	[M+H-H2O]+/[M+H-2H2O]+	2./2./	MS3/MS3	295.1368,193.1055,165.0737,139.0621,111.0450
20210711_medhora_rat_urine_metabolomics_MSMS_POS_20501.CDF	298.0994_0.95	5'-S-Methyl-5'-thioadenosine	Adenosine, 5'-S-methyl-5'-thio-	[M+H]+	2	MS2	298.1488,136.0624
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16703.CDF	299.129_5.13	Tetrahydrofolic acid	Tetrahydropteroylglutamic acid	[M+H-C5H9NO4]+	2	MS2	299.1329,149.0621,130.0655,121.0679,108.0542,105.0709,85.0293
20210704_medhora_rat_urine_metabolomics_MSMS_POS_07203.CDF	299.2012_6.02	4-Ketoretinal	Retinal, 4-oxo-	[M+H]+	2	MS2	299.1281,159.0833,141.0673,131.0583,115.0504,102.0922
20210711_medhora_rat_urine_metabolomics_MSMS_POS_05104.CDF	299.3071_7.09	Prostaglandin K1/DELTA-12-Prostaglandin D2		[M+H-H2O]+/[M+H-H2O]+	1./2.	MS3/MS2	299.2217,253.1849,155.0850
20210711_medhora_rat_urine_metabolomics_MSMS_POS_10401.CDF	300.0885_0.56	8-Hydroxyguanosine		[M+H]+	1	MS2	300.0932,283.1788,169.0177,151.0843,140.0819,136.0620,126.0581,113.0473
20210704_medhora_rat_urine_metabolomics_MSMS_POS_02003.CDF	300.2185_5.47	Protein Kinase C Substrate		[M+4H]4+	1	MS2	300.2167,253.1147,241.1385,236.1269,130.0643,115.0530,99.0454,85.0295
20210711_medhora_rat_urine_metabolomics_MSMS_POS_19902.CDF	301.1066_3.04	Leukotriene C4	LTC4	[M+2H]2+	2	MS3	301.2077,259.1637,241.1733,213.0450,159.0919
20210711_medhora_rat_urine_metabolomics_MSMS_POS_14102.CDF	301.2134_2.79	9-cis-Retinoic acid/4-Ketoretinol		[M+H]+/[M+H]+	1./2.	MS2/MS2	301.2045,241.1600,159.0920,105.0397,81.0707
20210711_medhora_rat_urine_metabolomics_MSMS_POS_14502.CDF	302.1994_2.87	Linoleoylglycine	N-9Z,12Z-1-Oxooctadecadien-1-ylglycine	[M+H-H2O]+	1	MS2	302.1979,285.1322,259.1636,241.1503,196.1689,159.0920,120.0804,95.0866
20210711_medhora_rat_urine_metabolomics_MSMS_POS_04302.CDF	303.1026_2.29	18-Carboxydinorleukotriene B4/Acetyl coenzyme A	/Acetyl CoA	[M+H-H2O]+/[M+H]+	1./1.	MS3/MS3	303.2041,285.1316,257.0923,243.1249,215.0853,195.0860,159.0922,
20210711_medhora_rat_urine_metabolomics_MSMS_POS_13403.CDF	303.1327_4.73	Acetyl coenzyme A	Coenzyme A, S-acetate	[M+H-C10H16O13N5P3]+	2	MS2	303.1377,271.0635,261.1133,215.1047,191.1061,161.0889
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16103.CDF	305.1874_5.04	1,25-Dihydroxy Vitamin D2/15S-Hydroperoxy-11Z,13E-eicosadienoic acid	/15(S)-HpEDE	[M+H-3H2O]+/[M+H-H2O]+	1./1.	MS3/MS3	305.1960,247.1816,209.0986,182.1161,145.0771,131.0560
20210711_medhora_rat_urine_metabolomics_MSMS_POS_20303.CDF	305.1934_5.36	6β-Hydroxytestosterone	6β,17β-Androst-4-en-3-one	[M+H]+	2	MS2	305.1969,247.1779,201.0563,182.1174,145.0712
20210711_medhora_rat_urine_metabolomics_MSMS_POS_07603.CDF	308.1056_4.46	N-Glycolylneuraminic acid/L-Glutathione, reduced		[M+H-H2O]+/[M+H]+	1./2	MS2/MS2	308.1089,197.0641,170.0612,155.0094,123.0449,85.0293
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16901.CDF	311.1015_0.76	21-Deoxycortisol	21-Deoxyhydrocortisone	[M+H]+	1	MS2	311.1599,295.1295,267.1301,223.1330,181.0875,141.0672,125.0479
20210711_medhora_rat_urine_metabolomics_MSMS_POS_05401.CDF	313.1416_0.36	(6S)-5-Methyltetrahydrofolic acid	Levomefolic acid	[M+H-C5H9O4N]+	1	MS2	313.1359,180.0886,139.0730,126.0596,109.0667
20210704_medhora_rat_urine_metabolomics_MSMS_POS_03603.CDF	313.2179_5.52	17α-Hydroxyprogesterone	Pregn-4-ene-3,20-dione, 17-hydroxy-	[M+H-H2O]+	1	MS2	313.2045,295.2059,185.1201,173.1319,159.0996,147.1156,133.1019,119.0864
20210711_medhora_rat_urine_metabolomics_MSMS_POS_13704.CDF	313.2755_8.5	1-Palmitoyl-2-linoleoyl-rac-glycerol		[M+H-C28H50O2]+	2	MS2	313.2749,196.9728
20210704_medhora_rat_urine_metabolomics_MSMS_POS_07003.CDF	315.1976_5.99	all-trans-4-Ketoretinoic acid		[M+H]+	1	MS2	315.2309,297.2200,279.2093,269.1889,254.1345,187.1405,173.1324,161.1303,147.1167,133.1023,109.0863,
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09503.CDF	315.2321_6.25	7,8-Dehydropregnenolone	Pregna-5,7-dien-20-one, 3-hydroxy-, (3β,9β)-	[M+H]+	1	MS2	315.2314,297.2204,273.2181,251.1777,209.1314,173.1327,147.1173,121.1017,95.0866
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_14101.CDF	318.1923_0.68	Adrenosterone/Leukotriene F4	Androst-4-ene-3,11,17-trione/LTF4	[M+NH4]+/[M+H-H2O]+	2./1.	MS2/MS4	318.1918,241.1079,211.0888,97.0851
20210711_medhora_rat_urine_metabolomics_MSMS_POS_05403.CDF	321.0958_4.42	N-Succinyl-5-aminoimidazole-4-carboxamide ribose		[M+H-3H2O]+	2	MS2	321.1094,259.0003,241.0761,213.0807,179.0426,147.9802,127.9959,
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_06701.CDF	322.0427_0.48	Cytidine 5'-monophosphate	5'-Cytidylic acid	[M-H]-	2	MS2	322.0487,193.0341,152.9833,109.0292,96.9599,78.9592,
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03703.CDF	325.2012_5.52	17-Keto-4(Z),7(Z),10(Z),13(Z),15(E),19(Z)-docosahexaenoic acid/Leukotriene B3	/5S,12R-Dihydroxy-6Z,8E,10E-eicosatrienoic acid	[M+H-H2O]+/[M+Na]+	1./2	MS2/MS3	325.2000,298.1315,268.1729,253.1863,229.1148,195.0897,165.0965
20210711_medhora_rat_urine_metabolomics_MSMS_POS_20403.CDF	327.2136_5.36	17-Hydroxy-4Z,7Z,10Z,13Z,15E,19Z-docosahexaenoic acid/Hydrocortisone	/(±)17-HDoHE	[M+H-H2O]+/[M+H-2H2O]+	1./2	MS2/MS2	327.1973,241.0850,190.1010
20210704_medhora_rat_urine_metabolomics_MSMS_POS_07801.CDF	328.1043_1.38	20-Hydroxy-N-arachidonoyltaurine		[M+H]+	1	MS4	328.1773,310.1262,246.0050,221.0192,208.0337,202.9980,194.0974,185.0788,126.0924
20210704_medhora_rat_urine_metabolomics_MSMS_POS_06903.CDF	328.2501_5.98	10-Nitrooleic acid	9-Octadecenoic acid, 10-nitro-, (9E)-	[M+H]+	1	MS2	328.1213,313.2093,298.1308,285.1587,268.2631,257.1253,241.0910,174.9990,159.0882,109.1016
20210711_medhora_rat_urine_metabolomics_MSMS_POS_06902.CDF	329.1576_2.53	Adrenorphin, free acid		[M+3H]3+	2	MS2	329.1114,314.1350,288.1480,271.1412,246.0070,202.9897
20210704_medhora_rat_urine_metabolomics_MSMS_POS_05803.CDF	329.1848_5.74	3β,5β-Tetrahydrocortisone	5β-Pregnan-3β,17α,21-triol-11,20-dione	[M+H-H2O]+	1	MS3	329.1987,311.1912,271.1976,253.1928,233.1060,203.1073,171.1172,147.1172,109.1020,
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09603.CDF	333.243_6.25	Cortol	Pregnane-3,11,17,20,21-pentol, (3α,5α,11β,20S)-	[M+H-2H2O]+	1	MS2	333.2336,315.2295,297.2196,273.2196,255.2096,209.1334,161.1308,121.1018,95.0869
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20602.CDF	334.0257_3.39	Nicotinic acid mononucleotide	Pyridinium, 3-carboxy-1-(5-O-phosphono-β-D-ribofuranosyl)-, inner salt	[M-H]-	2	MS2	334.0099,290.0395,193.0354,175.0242,122.0240
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_02301.CDF	335.0494_0.31	S-Nitroso-L-glutathione	N-(N-L-γ-Glutamyl-S-nitroso-L-cysteinyl)glycine	[M-H]-	2	MS2	335.1302,227.0992,160.0396,158.0763
20210704_medhora_rat_urine_metabolomics_MSMS_POS_06702.CDF	336.216_3.61	TRH Precursor Peptide		[M+3H]3+	2	MS2	336.1594,177.0352,159.0740,141.0342,122.0653,107.0543,95.0767,85.0214
20210711_medhora_rat_urine_metabolomics_MSMS_POS_15701.CDF	337.0842_0.72	Prostaglandin D3	9S,15S-Dihydroxy-11-oxo-5Z,13E,17Z-prostatrienoic acid	[M+Na]+	1	MS4	337.0949,199.0218,165.0109,148.9959
20210711_medhora_rat_urine_metabolomics_MSMS_POS_04404.CDF	337.1063_6.96	Biocytin	epsilon-N-Biotinyl-L-lysine	[M+H]+	1	MS4	337.1333,319.2412,227.1422,209.1326,183.1172
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01204.CDF	337.2528_6.42	Nutriacholic acid		[M+H-3H2O]+	1	MS2	337.2493,319.2401,293.2087,281.1698,227.1452,209.1329,169.0960,85.0282
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01803.CDF	341.1813_5.44	Coenzyme Q2	2,3-Dimethoxy-5-geranyl-6-methyl-1,4-benzoquinone	[M+Na]+	2	MS2	341.2910,325.1490,296.1286,279.9578,170.9981
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01304.CDF	344.2826_6.42	Lauroyl-L-carnitine	C12 Carnitine	[M+H]+	2	MS2	344.2479,183.1312,85.0579
20210704_medhora_rat_urine_metabolomics_MSMS_POS_04703.CDF	345.2068_5.61	19,20-Dihydroxy-4Z,7Z,10Z,13Z,16Z-docosapentaenoic acid/24,25-Dihydroxyvitamin	19,20-DiHDPA/24S,25-Dihydroxycholecalciferol	[M+H]+/[M+H-3H2O]+	1./1.	MS3/MS3	345.2046,327.1999,271.1868,259.1318,231.0359,151.0762
20210704_medhora_rat_urine_metabolomics_MSMS_POS_06603.CDF	347.2222_5.91	Corticosterone	11β,21-Dihydroxyprogesterone	[M+H]+	1	MS2	347.2187,329.2090,271.2043,253.1939,135.1132,121.1017
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01903.CDF	347.2226_5.44	Corticosterone	11β,21-Dihydroxyprogesterone	[M+H]+	1	MS2	347.2187,329.2105,301.2153,283.2053,267.2071,253.1953,145.1020,109.0992
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03604.CDF	347.2227_6.55	Cortodoxone	11-Deoxycortisol	[M+H]+	1	MS2	347.2227,329.2123,311.2026,287.1976,269.1914,163.1108
20210704_medhora_rat_urine_metabolomics_MSMS_POS_04802.CDF	349.0265_3.34	Thymidine 3',5'-cyclic monophosphate	Cyclic 3',5'-thymidylic acid	[M-H+2Na]+	2	MS2	349.0222,284.0446,203.9943,200.9748,181.0098,149.0976
20210711_medhora_rat_urine_metabolomics_MSMS_POS_06302.CDF	349.1826_2.46	11-Dehydrothromboxane B3/5S,12R-Dihydroxy-6Z,8E,10E,14Z-eicosatetraene-1,20-	/20-Carboxyleukotriene B4	[M+H-H2O]+/[M+H-H2O]+	2./2	MS2/MS2	349.1845,286.1963,174.0916,164.0659,97.0629
20210704_medhora_rat_urine_metabolomics_MSMS_POS_03803.CDF	349.2381_5.52	5β-Pregnan-3α,17,20β,21-tetrol-11-one	β-Cortolone	[M+H-H2O]+	1	MS2	349.2210,331.2244,313.2169,283.2069,271.2080,253.1944,211.1465,175.1400,145.1026,121.1014,95.0862
20210711_medhora_rat_urine_metabolomics_MSMS_POS_12503.CDF	349.2385_4.71	Allo-3α-tetrahydrocortisol	5α-Pregnane-3α,11β,17α,21-tetrol-20-one	[M+H-H2O]+	1	MS2	349.2377,331.2248,313.2170,301.2176,289.2152,269.1827,251.1748
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_02401.CDF	351.0572_0.31	Vitamin C	L-Ascorbic acid	[2M-H]-	2	MS2	351.0540,307.0429,289.0322,115.0021
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09903.CDF	353.2484_6.39	7-Keto-3α,12-α-dihydroxycholanic acid	Cholan-24-oic acid, 3,12-dihydroxy-7-oxo-, (3α,5β,12α)-	[M+H-3H2O]+	1	MS2	353.2434,335.2372,317.2260,307.2378,299.2018,283.1975,271.1689,259.1702,247.1701,235.1533,223.1493,209.1340,197.1334,181.1193,159.1183,145.1026,119.0870,95.0871,81.0710
20210704_medhora_rat_urine_metabolomics_MSMS_POS_04001.CDF	355.0814_1.21	Glutathione, oxidized	GSSG	[M+H-C10H14O6N2]+	1	MS2	355.0660,298.0925,200.9726,189.0644,179.0479,159.0322,155.0730,122.0693,113.0273
20210704_medhora_rat_urine_metabolomics_MSMS_POS_08403.CDF	355.264_6.06	Cholic acid		[M+H-3H2O]+	1	MS2	355.2645,319.2429,287.2013,263.1794,239.1804,199.1491,171.1181,145.1026,119.0870,95.0870,67.0562
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01604.CDF	357.2713_6.42	3β-Hydroxy-5-cholenoic acid		[M+H-H2O]+	1	MS2	201.1588,339.2455,247.1656,215.1708,185.1327,171.1159,157.1010,143.0850,119.0856,95.0865
20210704_medhora_rat_urine_metabolomics_MSMS_POS_05403.CDF	361.2016_5.71	Aldosterone	18-Oxocorticosterone	[M+H]+	1	MS2	361.1944,315.1959,297.1823,285.1830,267.1679,235.1051,169.0993
20210711_medhora_rat_urine_metabolomics_MSMS_POS_10202.CDF	362.0856_2.61	S-Lactoylglutathione		[M+H-H2O]+	2	MS2	362.1134,305.1548,282.9575,220.0271,187.0567,153.0542,
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_23802.CDF	363.075_3.91	1-Methyluric acid	Uric acid, 1-methyl-	[2M-H]-	2	MS2	363.0779,181.0880,166.0182,122.0280,80.9651
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_13303.CDF	373.2588_5.77	Isodeoxycholic acid	5β-Cholanic acid, 7α,12α-dihydroxy-	[M-H-H2O]-	2	MS2	373.1805,355.2489,331.1905,297.1127,259.0730,247.1149,231.1293,179.0992,153.1255
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01804.CDF	374.2779_6.42	N-Arachidonoyl-L-serine		[M+H-H2O]+	1	MS2	374.2686,269.2096,243.1713,199.1484,185.1325,171.1169,157.1014,143.1861,129.0713,117.0715,91.0548,81.0704
20210711_medhora_rat_urine_metabolomics_MSMS_POS_14903.CDF	376.2696_4.86	N-Arachidonoyl-L-alanine		[M+H]+	1	MS2	376.1378,202.1136,133.0709
20210711_medhora_rat_urine_metabolomics_MSMS_POS_13002.CDF	377.1466_2.72	(-)-Riboflavin	Vitamin B2	[M+H]+	1	MS2	377.1468,359.1356,243.0885,198.0665,172.0878,99.0446
20210704_medhora_rat_urine_metabolomics_MSMS_POS_01301.CDF	381.0092_1.03	Geranyl pyrophosphate	Diphosphoric acid, P-[(2E)-3,7-dimethyl-2,6-octadien-1-yl]-	[M-2H+3Na]+	2	MS2	381.0810,293.1054,267.1260,135.0814
20210711_medhora_rat_urine_metabolomics_MSMS_POS_12701.CDF	381.0802_0.64	Flavine mononucleotide	Riboflavin 5'-(dihydrogen phosphate)	[M+Na]+	2	MS3	381.0812,364.1391,295.0775,252.0736,221.0148,
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01501.CDF	381.0805_0.29	Flavine mononucleotide	Riboflavin 5'-(dihydrogen phosphate)	[M+Na]+	2	MS3	381.0807, 364.1400, 339.1055, 252.0734, 234.0620, 221.0138, 196.8751
20210711_medhora_rat_urine_metabolomics_MSMS_POS_11903.CDF	389.2309_4.67	Corticosterone 21-acetate/Palmitoleoyl 3-carbacyclic phosphatidic acid	Pregn-4-ene-3,20-dione, 21-(acetyloxy)-11-hydroxy-, (11β)-	[M+H]+/[M+H]+	1./1.	MS2/MS2	389.2295,371.2197,311.2009,285.2068,269.1857,237.0849,211.1311,185.1285,157.0981,131.0843,105.0705
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09302.CDF	391.1593_3.81	4-Androsten-17β-ol-3-one sulfate	Testosterone 17-sulfate	[M+Na]+	2	MS2	391.1582,311.1999,293.1819,217.0907
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_15001.CDF	393.13_0.86	3,4-Dihydroxy-L-phenylalanine	L-Dopa	[2M-H]-	2	MS2	393.0803,179.0334,135.0082,109.0302
20210711_medhora_rat_urine_metabolomics_MSMS_POS_15002.CDF	393.2109_2.92	1-Palmitoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol)	16:0 Lyso PG	[M+H-H2O]+	2	MS4	393.2093,313.2032
20210711_medhora_rat_urine_metabolomics_MSMS_POS_17704.CDF	393.2992_9.14	Chenodeoxycholic acid/1,25-Dihydroxy Vitamin D2	Cholan-24-oic acid, 3,7-dihydroxy-, (3α,5β,7α)-	[M+H]+/[M+H-2H2O]+	2./2.	MS2/MS2	393.2977,195.1219,174.9963,159.0011,
20210711_medhora_rat_urine_metabolomics_MSMS_POS_16203.CDF	397.1848_5.04	3-Oxo-4-cholestenoic acid		[M+H]+	2	MS3	397.2502,299.2347,269.1735,229.0914,211.0800,193.0612
20210711_medhora_rat_urine_metabolomics_MSMS_POS_11504.CDF	399.311_8.26	3β-Hydroxy-5-cholestenoic acid		[M+H-H2O]+	2	MS3	399.3090,299.1624,283.2631,199.0740,143.0137
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_17203.CDF	403.2458_6.03	1-O-(9Z-Octadecenyl)-sn-glycero-2,3-cyclic-phosphate	C18:1 Cyclic LPA	[M-H]-	2	MS2	403.2080,335.1841,123.0347,96.9598
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19603.CDF	405.2642_6.4	3-Oxocholic acid	3-Dehydrocholic acid	[M-H]-	1	MS2	405.2641,361.2749,343.2634,289.2161,271.1973,233.1770,195.1692,69.0351
20210704_medhora_rat_urine_metabolomics_MSMS_POS_08603.CDF	412.2859_6.07	Glycocholic acid	N-Choloylglycine	[M+H-3H2O]+	1	MS2	412.2840,337.2519,319.2423,295.2287,241.1860,227.1398,213.1620,199.1476,185.1277,158.0817,119.0864
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_13603.CDF	413.2002_5.82	5α-Pregnane-3α,17α-diol-20-one	PDIOL-S	[M-H]-	2	MS2	413.2001,96.9601
20210711_medhora_rat_urine_metabolomics_MSMS_POS_01503.CDF	413.2035_4.19	17β-Estradiol 3-β-D-glucuronide	1,3,5(10)-Estratriene-3,17β-diol 3-glucuronide	[M+H-2H2O]+	1	MS2	413.2131,367.1884,338.1195,255.0646,227.0593,209.0450,173.1090,159.1136,145.0994,131.0848,119.0840,105.0705,81.0705
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19003.CDF	417.2248_6.26	1-Oleoyl-L-α-lysophosphatidic acid	1-Oleoyl lysophosphatidic acid	[M-H-H2O]-	2	MS2	417.2230,349.2367
20210711_medhora_rat_urine_metabolomics_MSMS_POS_18904.CDF	419.3167_9.49	1-Oleoyl-sn-glycero-3-phosphoethanolamine	18:1 Lyso PE	[M+H]+	2	MS3	419.3612,265.1924,153.0732
20210704_medhora_rat_urine_metabolomics_MSMS_POS_10101.CDF	423.0935_1.65	Creatine phosphate	N-(Phosphonoamidino)sarcosine	[2M+H]+	2	MS2	423.1601,307.0603,293.1102,282.9691
20210704_medhora_rat_urine_metabolomics_MSMS_POS_09402.CDF	427.1809_3.81	Hydrocortisone 21-hemisuccinate	Cortisol, 21-(hydrogen succinate)	[M+H-H2O]+	2	MS3	427.1855,409.1756,265.1861,211.0676,199.0757,181.0651,171.0785,157.0649
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_24002.CDF	442.1619_3.94	Dihydrofolic acid	7,8-Dihydro-L-folic acid	[M-H]-	1	MS2	442.1613,203.0195,175.0247,159.0389,133.0286,117.0080,85.029359.0140
20210711_medhora_rat_urine_metabolomics_MSMS_POS_02004.CDF	447.2503_6.42	Epitestosterone glucuronide		[M+H-H2O]+	1	MS2	447.2496,430.2916,411.2726,317.2234,253.1577,227.1444,199.1490,183.1165
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_26901.CDF	456.0255_1.68	Chondroitin disaccharide 4-sulfate	Glycan Chondroitin 4-sulfate	[M-H]-	2	MS2	456.0303,412.0319,358.0523,279.9890,217.9666,172.9905
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_05703.CDF	461.145_5.14	Disialyllactose	GD3 ganglioside sugar	[M-2H]2-	1	MS2	461.1419,272.0677,151.0326,129.0186,121.0366,113.0241,95.0143,85.0291,71.0136
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_18003.CDF	464.3007_6.08	Glycocholic acid	N-Choloylglycine	[M-H]-	2	MS2	464.3006,446.2788,420.2784,402.2995,382.2664,95.0162,72.0245
20210704_medhora_rat_urine_metabolomics_MSMS_POS_07703.CDF	464.301_6.02	Tauroursodeoxycholic acid		[M+H-2H2O]+	1	MS2	464.2943,253.1621,227.1450,211.1515,199.1468,181.1051,167.0719,157.1002
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_02002.CDF	480.9954_2.05	Thymidine 5'-triphosphate	Thymidine 5'-(tetrahydrogen triphosphate)	[M-H]-	2	MS2	480.9944,401.0355,274.9795
20210711_medhora_rat_urine_metabolomics_MSMS_POS_04502.CDF	484.108_2.29	Glutathione, oxidized	GSSG	[M+H-C5H7O3N]+	2	MS2	484.0744,355.0908,338.0717,308.0624,271.0396,233.0396,233.0379,199.0283,191.0041
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20603.CDF	491.2393_6.43	Adrenorphin, free acid		[M-2H]2-	2	MS2	491.2263,449.1622,427.1833,316.1972,175.0250,113.0240,85.0284
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_14103.CDF	514.2828_5.9	Taurocholic acid		[M-H]-	2	MS2	514.2804,126.0243
20210711_medhora_rat_urine_metabolomics_MSMS_POS_12401.CDF	576.1295_1.68	BNP (1-32), rat		[M+6H]6+	2	MS2	576.1338,327.1017,309.0884,210.0446
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_18703.CDF	653.2609_6.16	Coproporphyrin I		[M-H]-	1	MS2	653.2620,565.2811,521.2973,223.0861
20210711_medhora_rat_urine_metabolomics_MSMS_POS_03204.CDF	701.499_6.51	Tetrahydrodeoxycortisol	5β-Pregnane-3α,17α,21-triol-20-one	[2M+H]+	2	MS2	701.4958,333.2429,315.2321
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_01504.CDF	271.2279_8.25	DL-3-Hydroxypalmitic acid	3-Hydroxy C16:0 FFA	[M-H]-	2	MS2	271.2256, 225.2209,
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_02802.CDF	290.0012_2.08	[illegible]	N-Acetylneuraminyllactose	[M-H]-	2	MS3	290.0705, 210.0807, 151.0387, 150.0125, 121.0786

20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19001.CDF	150.0555_1.2	DL-Norepinephrine	DL-Noradrenaline	[M-H-H2O]-	2	MS2	150.0302, 149.0401, 123.0518	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19101.CDF	172.991_1.2	trans-Aconitic acid/Citric acid	(E)-1-Propene-1,2,3-tricarboxylic acid	[M-H]-/[M-H-H2O]-	1./1.	MS2/MS2	172.9909, 129.0206, 111.0081, 85.0288	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19201.CDF	230.0124_1.2	Pyridoxamine 5-phosphate		[M-H-NH3]-	1	MS2	230.0121, 212.0922, 150.0552, 135.0442, 122.0293, 107.0494, 96.9598, 80.9707	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19502.CDF	195.0633_3.25	D-Gluconic acid	Pentahydroxycaproic acid	[M-H]-	1	MS2	195.0517, 119.0501, 99.0092	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_19802.CDF	241.1077_3.26	20-Hydroxy-4Z,7Z,10Z,13Z,16Z,18E-docosahexaenoic acid/D-myo-Inositol-1,2-	(±)20-HDoHE/	[M-H-C3H6O]-//[M-H]-	1./1.	MS3/MS3	241.1066, 226.1091, 225.1110, 200.1197, 197.112, 195.0629, 175.0978, 173.0815, 172.0969, 169.0830, 156.1170, 153.1155, 143.0686, 141.0558, 135.0808, 130.0870, 129.0855, 128.0385, 127.0757, 123.0803, 119.0496, 115.0732,	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20002.CDF	215.092_3.27	3-Oxo-1,8-octanedicarboxylic acid/13,14-Dihydro-15-ketoprostaglandin J2	Decanedioic acid, 4-oxo-/11,15-Dioxoprosta-5Z,9-en-1-oic acid	[M-H]-/[M-H-H2O]-	1./1.	MS2/MS2	215.0955, 153.0915, 135.0465, 123.0397, 80.9648	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20303.CDF	407.2799_6.43	Ursocholic acid	Cholan-24-oic acid, 3,7,12-trihydroxy-, (3α,5β,7β,12α)-	[M-H]-	1	MS2	407.2800, 389.2673, 371.2562, 363.2174, 361.2015, 353.2459, 345.2787, 343.2636, 341.2436, 329.1812, 327.2659, 325.2659, 325.2525, 323.2149, 317.2087, 301.2162, 293.2148, 289.2160, 217.1570, 96.9607, 69.0342	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20701.CDF	188.0349_1.26	Kynurenic acid	2-Quinolinecarboxylic acid, 4-hydroxy-	[M-H]-	1	MS2	188.0170, 144.0450	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20801.CDF	285.0613_1.28	N-Acetylaspartylglutamic acid	Spaglumic acid (NAAG)	[M-H-H2O]-	2	MS2	285.0657, 113.0245, 112.0376, 129.0309, 96.0333	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_20802.CDF	163.0395_3.42	**L-Tyrosine/p-Hydroxyphenyllactic acid**	L-Phenylalanine, 4-hydroxy-/	[M-H-NH3]-/[M-H-H2O]-	1./1.	MS2/MS2	163.0488, 162.0558, 119.0500	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_21001.CDF	307.0437_1.28	2'-Deoxyuridine 5'-monophosphate	2'-Deoxyuridylic acid (dUMP)	[M-H]-	1	MS2	307.0246, 264.0066, 246.0224, 194.9960, 176.9652, 111.0127	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_21201.CDF	258.0426_1.31	D-Glucosamine, 6-sulfate	D-Glucose, 2-amino-2-deoxy-, 6-(hydrogen sulfate)	[M-H]-	2	MS2	28.0071, 199.0184, 181.0503, 138.0632, 79.0136	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_21901.CDF	151.0399_1.38	4-Hydroxyphenylacetic acid	4,3-Cresotic acid	[M-H]-	1	MS2	11.0396, 123.0442, 109.0290, 107.0496, 91.0190	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_21902.CDF	446.1932_3.56	1-Decanoyl-2-hydroxy-sn-glycero-3-phosphocholine	10:0 Lyso PC	[M+Cl]-	2	MS2	446.1930, 224.0458	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_22003.CDF	389.1967_6.57	13,14-Dihydro-16,16-difluoroprostaglandin D2/α-Muricholic acid		[M-H]-/[M-H]-	2./2.	MS2/MS3	389.1969, 315.2542, 307.1154, 289.1117, 287.9918, 247.0610, 245.1447, 221.0731, 216.9889, 207.0357,	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_22502.CDF	183.102_3.6	Isopentenyl pyrophosphate	Diphosphoric acid, P-(3-methyl-3-buten-1-yl) ester	[M-H-H2O]-	2	MS3	183.0732, 165.0543, 139.0716, 137.0604, 125.0967	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_22602.CDF	201.1126_3.6	Sebacic acid/15-Hydroperoxy-5Z,8Z,11Z,13E,17Z-eicosapentaenoic acid	Decanedioic acid/15-HpEPE	[M-H]-/[M-H-H2O]-	1./1.	MS2/MS4	201.0229, 183.0987, 139.1118, 137.0948, 123.0714, 82.9610	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_23001.CDF	203.0015_1.49	Prostaglandin K2	9,11-Dioxo-15S-hydroxy-5Z,13E-prostadienoic acid	[M-H-H2O]-	2	MS4	203.0012, 187.9996, 172.9961, 160.0398, 159.0333, 147.0324,	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_23301.CDF	279.9893_1.55	Uridine 5'-diphosphoglucuronic acid		[M-H-C6H9O9P]-	2	MS3	279.0134, 243.9067, 235.1077, 196.9872, 182.0260, 169.0138, 153.9944, 151.0397, 136.0522	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_23602.CDF	343.0856_3.88	3α,7α-Dihydroxy-12-oxocholanoic acid	12-Ketochenodeoxycholic acid	[M-H-H2O]-	1	MS3	343.0895, 325.0891, 298.1032, 297.0091, 253.0454	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_23701.CDF	206.0452_1.62	3-Hydroxykynurenine	α,2-Diamino-3-hydroxy-?-oxobenzenebutanoic acid	[M-H-NH3]-	1	MS2	206.0424, 204.9821, 188.0360, 162.0555, 160.0395, 147.0308, 144.0352, 134.0589, 120.0451, 118.0247, 108.0222	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_24501.CDF	134.0608_1.67	Adenosine 2',3'-cyclic monophosphate	Cyclic 2',3'-AMP	[M-H-C5H7O6P]-	2	MS2	134.0393, 92.0266	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_26501.CDF	379.0909_1.68	3-Dehydroquinic acid		[2M-H]-	2	MS2	0	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_27901.CDF	230.1029_1.72	Suberylglycine	Octanoic acid, 8-[(carboxymethyl)amino]-8-oxo-	[M-H]-	1./	MS2	230.1026, 212.0915, 186.1127, 173.0047, 168.1021, 150.0555, 142.1225, 100.0759	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_28301.CDF	169.0138_1.79	2,3-Dinorthromboxane B1	9α,11,15S-Trihydroxy-2,3-dinorthromba-13E-en-1-oic acid	[M-H]-	1	MS3	169.0138, 151.0037, 125.0256, 123.0447, 109.0657	
20210717_medhora_rat_urine_metabolomics_MSMS_NEG_28901.CDF	193.0501_1.89	D-Galacturonic acid/D-Glucuronic acid		[M-H]-/[M-H]-	2./2.	MS2/MS2	193.0497, 149.0604, 133.0289, 75.0269	

Supplementary Table 3. List of dysregulated metabolites in rat urine quantified using targeted MRM-based LC MS analysis, following exposure to 13.0 Gy of X-ray radiation at 1d, 14d, 30d and 90 d and potential protection by three APC variants administered at 24h and 48h.

	13 Gy vehicle vs. 0 Gy vehicle																Human WT APC treatment vs. 13 Gy vehicle																Rat 3K3A APC treatment vs. 13 Gy vehicle			
	1d				14d				30d				90d				1d				14d				30d				90d				1d			
Metabolites	FC	log2(FC)	FDR	-log10p	FC	log2(FC)	FDR	-log10p	FC	log2(FC)	FDR	-log10p	FC	log2(FC)	FDR	-log10p	FC	log2(FC)	P.value	-log10p	FC	log2(FC)	P.value	-log10p	FC	log2(FC)	P.value	-log10p	FC	log2(FC)	P.value	-log10p	FC	log2(FC)	P.value	-log10p
1-METHYLADENOSINE_pos_1	0.90484	-0.14427	0.50367	0.29786	1.4217	0.50761	0.45917	0.33802	1.585	0.6645	0.066247	1.1788	0.4094	-1.2884	0.055374	1.2567	1.022	0.031402	0.65603	0.18308	0.94033	-0.088767	0.94052	0.026634	1.0629	0.088054	0.60696	0.21684	0.8844	-0.17724	0.53089	0.27499	1.2789	0.3549	0.2734	0.5632
1-METHYLNICOTINAMIDE_pos_1	1.3498	0.43278	0.022999	1.6383	0.80495	-0.31302	0.39155	0.40721	1.001	0.0013992	0.91736	0.037462	0.57598	-0.7959	0.0060172	2.2206	1.0187	0.026682	0.96284	0.016448	0.90228	-0.14835	0.36599	0.43654	1.0992	0.13649	0.45896	0.33823	1.0803	0.11139	0.49381	0.30644	0.94171	-0.086647	0.46225	0.33512
2,3-BUTANEDIOL_pos_1	0.6442	-0.63441	0.0043242	2.3641	1.3057	0.38479	0.33544	0.47438	1.6457	0.71868	0.0030029	2.5225	0.53836	-0.89336	0.014348	1.8432	1.2505	0.32253	0.10515	0.97818	1.0651	0.091031	0.50285	0.29856	0.93679	-0.094209	0.33648	0.47304	1.1373	0.18562	0.39909	0.39893	1.409	0.49469	0.0022267	2.6523
2-AMINOBUTYRIC ACID_pos_1	0.7044	-0.50554	0.0017102	2.767	1.1798	0.23856	0.40005	0.39788	1.1006	0.13823	0.55615	0.25481	0.39651	-1.3346	0.00014546	3.8373	0.97527	-0.03613	0.74313	0.12893	1.016	0.044814	0.53403	0.27243	1.1286	0.17458	0.1141	0.9427	0.99145	-0.012389	0.81746	0.087535	1.1493	0.20075	0.21257	0.67249
2-AMINOISOBUTYRATE_pos_1	0.73478	-0.44461	0.022412	1.6495	1.1275	0.17312	0.52393	0.28073	1.1114	0.15239	0.50335	0.29813	0.46378	-1.1085	0.0012822	2.892	0.9701	-0.043801	0.7588	0.11987	1.0315	0.044772	0.5911	0.22834	1.1292	0.17524	0.15201	0.81813	0.9636	-0.053494	0.60788	0.21618	1.1724	0.22946	0.23742	0.62447
2-AMINOOCTANOIC ACID_pos_1	0.47586	-1.0714	2.43E-05	4.6146	1.0604	0.084656	0.7322	0.13537	1.119	0.16225	0.34946	0.4566	0.62081	-0.68777	0.0096168	2.017	0.93485	-0.097191	0.67576	0.17021	0.99249	-0.010873	0.88912	0.051039	1.1178	0.16061	0.14803	0.82966	0.97526	-0.036148	0.70442	0.15217	1.1434	0.19337	0.43433	0.36218
2-HYDROXY-3-METHYLBUTYRIC ACID_neg_1	0.32016	-1.6431	4.51E-07	6.3461	0.91629	-0.12613	0.7327	0.13507	0.50072	-0.99792	0.00011117	3.954	1.7027	0.76785	0.0039115	2.4077	0.78889	-0.34211	0.081041	1.0913	0.92443	-0.11337	0.58965	0.22941	0.88272	-0.17997	0.22896	0.64024	1.0356	0.050526	0.70488	0.15188	1.03	0.042651	0.80114	0.096294
2-HYDROXY-3-METHYLBUTYRIC ACID_pos_4	1.7306	0.79124	0.0048638	2.313	1.2014	0.2647	0.54881	0.26058	1.1727	0.22978	0.48336	0.31573	0.50568	-0.98371	0.048661	1.3128	0.76351	-0.38928	0.070239	1.1534	0.80681	-0.30969	0.14148	0.84929	0.93994	-0.08936	0.48717	0.31232	0.85131	-0.23225	0.8493	0.070936	0.85566	-0.22488	0.19535	0.70919
2-HYDROXYBUTYRATE_neg_3	0.13504	-2.8885	6.71E-12	11.173	1.1641	0.21924	0.94304	0.02547	0.57609	-0.79563	0.018465	1.7336	0.83638	-0.25777	0.77938	0.10825	0.88314	-0.17929	0.1179	0.92848	0.95343	-0.068807	0.9734	0.011707	0.80449	-0.31386	0.19186	0.71702	0.99717	-0.0040922	0.66645	0.17624	1.014	0.019999	0.78957	0.10261
2-ISOPROPYLMALIC ACID_neg_2	0.14477	-2.7882	6.93E-08	7.159	1.2319	0.30091	0.56576	0.24737	0.94451	-0.082363	0.76089	0.11868	2.4738	1.3067	7.38E-05	4.1322	0.93666	-0.094398	0.54785	0.26134	1.0002	0.00033255	0.84489	0.073198	0.86812	-0.20403	0.20638	0.68534	0.87222	-0.19724	0.31596	0.50037	0.83267	-0.26418	0.3083	0.68131
2-KETOHEXANOIC ACID_neg_1	0.33627	-1.5723	2.62E-08	7.5817	1.2837	0.36026	0.29363	0.5322	0.79548	-0.3301	0.052353	1.2811	2.2758	1.1863	7.87E-05	4.1043	0.84665	-0.24017	0.13466	0.87077	0.86258	-0.21327	0.26124	0.58297	0.85928	-0.2188	0.11813	0.92763	1.0805	0.11169	0.36758	0.43465	1.014	0.1394	0.6277	0.20225
2-KETOHEXANOIC ACID_pos_2	1.3682	0.45229	0.049004	1.3098	0.95496	-0.066491	0.84075	0.075333	1.0558	0.078396	0.66327	0.17831	0.75079	-0.41352	0.12669	0.89727	0.97447	-0.037312	0.92104	0.03572	0.95198	-0.071	0.6547	0.18396	1.0813	0.11283	0.42077	0.37595	0.99825	-0.0025212	0.95597	0.019557	1.1056	0.14477	0.77642	0.1099
2-PHOSPHOGLYCERATE_pos_4	1.3766	0.46111	0.046374	1.3337	1.3775	0.46209	0.5532	0.25711	2.5165	1.3314	0.010889	1.963	0.45029	-1.1511	1.40E-05	4.854	1.018	0.025756	0.71407	0.14626	0.75281	-0.40964	0.27886	0.55462	0.9916	-0.012164	0.99949	0.00022142	0.96678	-0.048736	0.55172	0.25828	1.0964	0.13274	0.4343	0.36221
3-(4-HYDROXYPHENYL)PYRUVATE_neg_1	0.46285	-1.1114	0.00020877	3.6803	1.2571	0.33013	0.86623	0.062365	1.2869	0.36386	0.21646	0.66463	2.7583	1.4638	1.44E-06	5.8417	0.97805	-0.032016	0.94689	0.023701	1.0224	0.031942	0.60507	0.21819	0.80564	-0.3118	0.11195	0.95097	0.9822	-0.025904	0.67136	0.17304	1.2239	0.29148	0.67952	0.1678
3-AMINOISOBUTANOIC ACID_pos_1	0.51994	-0.94358	0.2985	0.52505	0.93111	-0.10297	0.85309	0.069007	1.1753	0.23301	0.49069	0.30444	0.91624	-0.12621	0.85105	0.070044	0.52326	-0.93441	0.10412	0.98247	0.94066	-0.088261	0.61182	0.21338	1.0629	0.088021	0.72373	0.14043	0.74887	-0.41722	0.10484	0.97945	0.5613	-0.83316	0.11821	0.93476
3-HYDROXY-3-METHYLGLUTARYL-COA_+2_neg_3	3.9338	1.9759	0.0014247	2.8463	3.7388	1.9026	0.41329	0.38375	11.987	3.5834	0.00025947	3.5859	2.5146	1.3303	0.036513	1.4375	0.94857	-0.076176	0.89254	0.049374	0.90064	-0.15098	0.64696	0.18912	0.97961	-0.029719	0.85803	0.066497	1.0682	0.095183	0.36211	0.44115	1.6268	0.70202	0.15301	0.81527
3-HYDROXYANTHRANILIC ACID_pos_1	0.38612	-1.3729	0.00014496	3.8388	1.0754	0.10489	0.85309	0.069007	1.6383	0.71217	0.010889	1.963	0.43963	-1.1856	0.0065646	2.1828	1.0269	0.038358	0.58234	0.23482	1.0549	0.077127	0.67818	0.16865	0.96198	-0.055924	0.65639	0.18284	1.0995	0.13688	0.38826	0.41088	1.2773	0.35309	0.11986	0.92133
3-HYDROXYBUTYRYL-CoA_-2_neg_4	1.1254	0.17044	0.42862	0.36793	0.78292	-0.35306	0.41104	0.38611	0.71649	-0.48099	0.1108	0.95545	1.3064	0.38557	0.70956	0.14901	0.80122	-0.31973	0.064784	1.1885	0.66273	-0.59352	0.12577	0.90042	1.1129	0.15429	0.47674	0.32172	0.91197	-0.13294	0.8293	0.081287	1.049	0.068956	0.42263	0.37404
3-HYDROXYPHENYLACETIC ACID_neg_1	0.37118	-1.4298	4.88E-07	6.312	1.1513	0.2033	0.27183	0.56571	0.85751	-0.22177	0.14612	0.8353	2.2472	1.1681	2.36E-05	4.6279	0.74251	-0.42951	0.026913	1.57	0.93886	-0.091024	0.32476	0.48878	0.89365	-0.16222	0.17651	0.75324	1.0248	0.035373	0.81362	0.089577	0.99894	-0.0015244	0.80778	0.092709
3-METHYL-2-OXOVALERIC ACID_neg_1	0.68007	-0.55624	0.00039845	3.3996	1.0455	0.064257	0.77309	0.11177	0.66621	-0.58595	0.0086621	2.0624	3.0048	1.5873	1.25E-07	6.9047	0.90696	-0.14088	0.1384	0.85886	0.83037	-0.26818	0.027401	1.5622	0.83659	-0.25742	0.11707	0.93156	1.0163	0.023394	0.86318	0.063901	1.0045	0.0064795	0.65593	0.18314
3-METHYLHISTAMINE_pos_2	0.66342	-0.592	0.071865	1.1435	0.87114	-0.19902	0.6175	0.20936	1.5128	0.59721	0.19713	0.70524	0.65538	-0.60961	0.18954	0.72229	1.2451	0.31629	0.21164	0.6744	1.1435	0.1934	0.39897	0.39906	1.0231	0.032969	0.77383	0.11135	0.80929	-0.30526	0.53897	0.26843	1.3882	0.47323	0.21226	0.67313
4-AMINOBENZOIC ACID_pos_1	0.23893	-2.0653	9.16E-09	8.0379	1.331	0.4125	0.34	0.46852	1.3617	0.44537	0.092716	1.0328	0.53865	-0.89258	0.10368	0.98431	0.83183	-0.26564	0.13213	0.879	0.9561	-0.064769	0.7296	0.13691	1.0668	0.093261	0.53969	0.26786	0.81326	-0.29822	0.17185	0.76485	1.0304	0.043197	0.65545	0.18346
4-HYDROXYBENZOATE_neg_1	0.68167	-0.55286	0.0060044	2.2215	1.3607	0.4443	0.10596	0.97487	0.86338	-0.21193	0.22765	0.64273	2.9661	1.5686	1.00E-07	7.0002	0.70527	-0.50375	0.01706	1.7675	0.83934	-0.25267	0.16309	0.78757	0.88295	-0.1796	0.18669	0.72888	1.1102	0.15081	0.42431	0.37231	1.0527	0.074076	0.84513	0.073075
4-IMIDAZOLEACETATE_pos_1	1.1196	0.16297	0.29404	0.53159	0.94589	-0.080262	0.90156	0.045005	0.7234	-0.46713	0.027113	1.5668	0.47196	-1.0832	0.0091545	2.0384	1.0094	0.013548	0.95135	0.021658	0.98442	-0.022655	0.91972	0.036345	0.99875	-0.0018035	0.92015	0.03614	1.0233	0.033216	0.71235	0.14731	1.231	0.29981	0.045023	1.3466
4-PYRIDOXATE_neg_2	0.71434	-0.48532	0.051161	1.2911	1.5394	0.62237	0.013566	1.8676	0.87355	-0.19504	0.43753	0.359	3.579	1.8395	3.57E-06	5.4468	0.99819	-0.0026088	0.63179	0.19942	0.9588	-0.060705	0.65594	0.18313	0.9066	-0.14146	0.52928	0.27632	0.95478	-0.066761	0.85234	0.069385	1.5744	0.65477	0.024262	1.6151
4-PYRIDOXATE_pos_1	0.56173	-0.83205	0.015316	1.8149	1.4619	0.54786	0.060954	1.215	1.1903	0.25138	0.31112	0.50708	0.61992	-0.68984	8.09E-05	4.092	1.0805	0.11168	0.32146	0.49288	0.98181	-0.026478	0.82459	0.08376	1.0836	0.11587	0.42448	0.37214	1.0167	0.023945	0.99065	0.0040793	1.6116	0.68845	0.012957	1.8875
5-HYDROXYTRYPTOPHAN_neg_2	0.85872	-0.21975	0.52237	0.28202	1.7604	0.81591	0.37468	0.42634	2.6689	1.4162	7.30E-05	4.1365	4.0571	2.0205	1.64E-06	5.7853	0.83247	-0.26452	0.061009	1.2146	0.87809	-0.18755	0.79707	0.098502	0.90904	-0.13759	0.40888	0.3884	0.95645	-0.064231	0.51794	0.28572	1.0802	0.1113	0.79687	0.098611
5-HYDROXYTRYPTOPHAN_pos_1	1.531	0.61447	0.023834	1.6228	1.7011	0.76646	0.6902	0.16102	1.3169	0.39713	0.21717	0.6632	0.43967	-1.1855	0.024984	1.6023	1.0992	0.13645	0.50135	0.29986	0.69312	-0.52883	0.65668	0.18264	0.98393	-0.023376	0.5958	0.2249	0.99033	-0.014017	0.94894	0.022763	1.4466	0.53269	0.018935	1.7227
5-METHOXYTRYPTOPHAN_pos_2	0.68072	-0.55486	0.042592	1.3707	1.5241	0.60798	0.076679	1.1153	1.2835	0.36005	0.65373	0.1846	0.49384	-1.0179	0.12891	0.88971	0.96802	-0.046886	0.74382	0.12853	0.80797	-0.30762	0.22129	0.65504	1.1898	0.25067	0.63172	0.19947	1.04	0.056621	0.88256	0.054258	0.9883	-0.016977	0.69705	0.15674
5-THYMIDYLIC ACID_neg_1	1.5457	0.62829	0.0062274	2.2057	0.91025	-0.13566	0.64773	0.1886	0.92004	-0.12023	0.63798	0.19519	1.438	0.5241	0.024134	1.6174	0.89053	-0.16726	0.43569	0.36082	0.92472	-0.11291	0.27756	0.55664	0.87446	-0.19354	0.1374	0.862	0.99809	-0.0027597	0.98207	0.0078554	1.1714	0.22826	0.19386	0.71251
5-THYMIDYLIC ACID_pos_1	1.0588	0.082426	0.57021	0.24397	0.80795	-0.30766	0.94644	0.023906	0.89321	-0.16293	0.71859	0.14352	3.8996	1.9633	0.11406	0.94287	1.9465	0.96089	0.90763	0.042089	1.6299	0.7048	0.35406	0.45093	0.99052	-0.013745	0.64573	0.18995	0.41756	-1.2599	0.49557	0.30489	4.6371	2.2132	0.19629	0.70709
6-PHOSPHOGLUCONATE_pos_3	0.60974	-0.71374	0.18235	0.73909	1.4288	0.51477	0.46214	0.33523	1.606	0.68344	0.31298	0.50449	0.43928	-1.1868	0.20147	0.6958	1.7068	0.77132	0.69148	0.16022	1.1336	0.18089	0.71798	0.14389	1.61	0.68705	0.016364	1.7861	1.0408	0.057689	0.63886	0.1946	1.6629	0.73374	0.058343	1.234
7-METHYLGUANOSINE_pos_1	0.93256	-0.10073	0.50204	0.29926	1.5072	0.5919	0.10262	0.98876	1.4909	0.57615	0.043059	1.3659	0.6833	-0.5494	0.087068	1.0601	1.1303	0.17671	0.29027	0.53719	1.0049	0.007023	0.79785	0.09808	0.99934	-0.00095739	0.99553	0.0019455	0.90319	-0.14691	0.41469	0.38228	1.5987	0.67687	0.0064562	2.19
ACADESINE_neg_2	0.60616	-0.72222	0.00073334	3.1347	0.9872	-0.018583	0.96678	0.014673	0.95787	-0.0621	0.83342	0.079134	0.79586	-0.32941	0.26575	0.57553	0.82701	-0.27402	0.055138	1.2585	0.85479	-0.22635	0.21239	0.67287	0.9741	-0.03786	0.85472	0.068176	1.1732	0.23042	0.40656	0.39088	1.0768	0.10677	0.75175	0.12393



Supplementary Table 4a. List of dysregulated pathways in rat urine following exposure to 13.0 Gy of X-ray radiation at 1d, 14d, 30d and 90d.				
13 Gy vehicle vs. 0 Gy vehicle (p values)				
	d1	d14	d30	d90
Alanine, aspartate and glutamate metabolism	1.4347E-07	-	0.0036354	0.00003939
alpha-Linolenic acid metabolism	0.00041387	0.049357	-	0.00029328
Amino sugar and nucleotide sugar metabolism	-	-	-	0.030661
Aminoacyl-tRNA biosynthesis	0.000018211	0.00002466	0.00035083	0.00077749
Arginine and proline metabolism	0.00023656	0.0032839	0.013788	0.00053236
Arginine biosynthesis	1.3023E-06	-	0.0015199	0.000010228
Biosynthesis of unsaturated fatty acids	8.1909E-08	-	-	0.000025722
Butanoate metabolism	0.0031336	-	-	-
Citrate cycle (TCA cycle)	0.00031864	-	0.039332	0.00016591
Cysteine and methionine metabolism	0.0018492	-	-	0.018087
Glutathione metabolism	0.00056426	0.021712	-	0.0080464
Glycerolipid metabolism	-	-	-	0.012418
Glycerophospholipid metabolism	0.0086389	0.00021965	-	0.00047111
Glycine, serine and threonine metabolism	0.00036892	-	0.035851	0.00016642
Glycolysis / Gluconeogenesis	0.035989	-	-	0.0054767
Glyoxylate and dicarboxylate metabolism	0.00028559	-	-	0.00012798
Linoleic acid metabolism	-	0.01923	-	-
Pantothenate and CoA biosynthesis	0.0095811	0.01025	-	0.0061964
Pentose phosphate pathway	0.00061984	-	-	0.011979
Phenylalanine metabolism	0.031028	-	-	-
Phenylalanine, tyrosine and tryptophan biosynthesis	0.0014313	-	-	0.023581
Purine metabolism	6.4054E-09	-	0.00011953	4.7464E-08
Pyrimidine metabolism	1.8942E-10	0.040405	9.0641E-06	4.5175E-08
Pyruvate metabolism	0.018194	-	-	0.0022031
Riboflavin metabolism	0.028684	-	-	-
Sphingolipid metabolism	2.8286E-06	0.000041827	-	1.5317E-06
Taurine and hypotaurine metabolism	0.016123	-	-	0.012156
Valine, leucine and isoleucine biosynthesis	0.000088649	0.000025234	-	0.0010089
Valine, leucine and isoleucine degradation	-	0.0038086	-	0.013343
Aminosugars metabolism	-	0.007394337	0.015544912	-
Androgen and estrogen biosynthesis and metabolism	0.037559869	-	-	0.013024116
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	0.043357701	0.000168053
Beta-Alanine metabolism	-	0.017393496	-	-
Bile acid biosynthesis	-	-	-	0.007814469
Biopterin metabolism	-	0.026048231	-	-
Blood Group Biosynthesis	-	0.049827746	0.040836904	-
C21-steroid hormone biosynthesis and metabolism	-	0.002268717	-	8.40266E-05
Carnitine shuttle	-	-	-	0.014452567
Drug metabolism - cytochrome P450	0.047727082	-	0.005629779	-
Drug metabolism - other enzymes	-	0.049827746	0.039744559	-
Glutamate metabolism	-	0.048819427	-	-
Glycosphingolipid biosynthesis - ganglioseries	-	0.049827746	-	-
Glycosphingolipid biosynthesis - lactoseries	-	0.049827746	0.040836904	-
Glycosphingolipid biosynthesis - neolactoseries	-	0.049827746	0.040836904	-
Glycosphingolipid metabolism	-	0.048819427	-	-
Histidine metabolism	-	0.017393496	-	-
Keratan sulfate biosynthesis	-	0.049827746	0.040836904	-
Methionine and cysteine metabolism	-	-	-	0.028569028
Nitrogen metabolism	-	0.049827746	-	-
O-Glycan biosynthesis	-	0.049827746	0.040836904	-
Porphyrin metabolism	-	0.016385178	-	0.028569028
Putative anti-Inflammatory metabolites formation from EPA	-	0.017393496	-	-
Sialic acid metabolism	0.025544072	-	-	-
Squalene and cholesterol biosynthesis	-	0.030249559	-	-
Tryptophan metabolism	0.004033275	-	-	-
Tyrosine metabolism	0.001764558	0.031341904	0.001092345	-
Urea cycle/amino group metabolism	0.056801949	-	-	-
Vitamin B3 (nicotinate and nicotinamide) metabolism	-	0.049827746	-	-
Vitamin B6 (pyridoxine) metabolism	-	-	0.015544912	-

Supplementary Table 4b. List showing potential restoration of biological pathways in rat urine after APC (human WT, Rat 3K3A and rat WT) treatment at 24h and 48h post irradiation to 13.0 Gy of X-ray radiation at 1d, 14d, 30d and 90d.

	Human WT APC treatment vs. 13 Gy vehicle (p values)			Rat 3k3a APC treatment vs. 13 Gy vehicle (p values)			Rat WT APC treatment vs. 13 Gy vehicle (p values)		
	d14	d30	d90	d14	d30	d90	d14	d30	d90
1- and 2-Methylnaphthalene degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
3-Chloroacrylic acid degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
3-oxo-10R-octadecatrienoate beta-oxidation	0.00487354	0.018401815	0.043777834	-	0.045458365	0.022939249	-	0.034282833	-
Alanine and Aspartate Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Alkaloid biosynthesis II	0.00487354	0.024787833	0.046886816	-	0.045458365	0.022939249	-	0.048147215	-
alpha-Linolenic acid metabolism	0.03316	0.04129	0.03316	0.03316	0.049357	-	0.04129	0.03316	-
Aminoacyl-tRNA biosynthesis	-	-	-	-	-	0.0054168	-	-	0.0054168
Aminosugars metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.036383497	-	-
Androgen and estrogen biosynthesis and metabolism	0.00487354	-	0.046886816	0.023611461	0.045458365	0.022939249	-	0.02218301	0.035459205
Arachidonic acid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Arginine and Proline Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Ascorbate (Vitamin C) and Aldarate Metabolism	0.00487354	0.01462062	0.046886816	-	0.045458365	0.009495	-	0.004453407	-
Ascorbate and aldarate metabolism	-	0.025574	-	-	-	-	-	-	-
Aspartate and asparagine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Atrazine degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Benzoate degradation via CoA ligation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Beta-Alanine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Bile acid biosynthesis	0.00487354	-	0.046886816	0.000756239	0.045458365	0.022939249	-	-	0.002100664
Biopterin metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Blood Group Biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Butanoate metabolism	0.00487354	0.04898748	0.046886816	-	0.045458365	0.022939249	-	-	-
C21-steroid hormone biosynthesis and metabolism	0.00487354	-	0.036719603	0.002016637	0.045458365	0.022939249	-	0.000504159	0.046466683
C5-Branched dibasic acid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Caffeine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Carbon fixation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Carnitine shuttle	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.046382657	-	-
Chondroitin sulfate degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.021174691	-	-
CoA Catabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
D4&E4-neuroprostanes formation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
De novo fatty acid biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	0.008654735
Dimethyl-branched-chain fatty acid mitochondrial beta-oxidation	0.00487354	0.017141417	0.046886816	-	0.045458365	0.022939249	-	-	-
Di-unsaturated fatty acid beta-oxidation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Drug metabolism - cytochrome P450	0.00487354	-	0.000504159	0.044281993	0.045458365	0.022939249	-	-	-
Drug metabolism - other enzymes	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Dynorphin metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Electron transport chain	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Fatty acid activation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	0.002100664
Fatty Acid Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Fatty acid oxidation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Fatty acid oxidation, peroxisome	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Fructose and mannose metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Galactose metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.047895135	-	-
Geraniol degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glutamate metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glutathione Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycerolipid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycerophospholipid metabolism	0.0030573	0.00011161	0.000045368	0.000045368	0.0074218	0.00059553	0.00011161	0.000045368	0.00059553
Glycine, serine, alanine and threonine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycolysis and Gluconeogenesis	0.00487354	0.018821948	0.046886816	-	0.045458365	0.022939249	-	0.032014116	-
Glycosaminoglycan degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycosphingolipid biosynthesis - ganglioseries	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycosphingolipid biosynthesis - globoseries	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycosphingolipid biosynthesis - lactoseries	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycosphingolipid biosynthesis - neolactoseries	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glycosphingolipid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.036383497	-	0.042433409
Glycosylphosphatidylinositol (GPI)-anchor biosynthesis	-	0.044409	0.035677	0.035677	-	-	0.044409	0.035677	-
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Glyoxylate and Dicarboxylate Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Heparan sulfate biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Heparan sulfate degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.021174691	-	-
Hexose phosphorylation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Histidine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Hyaluronan Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Keratan sulfate biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Keratan sulfate degradation	0.00487354	-	0.043777834	-	0.045458365	0.022939249	0.015796992	-	-
Leukotriene metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Limonene and pinene degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Linoleate metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Linoleic acid metabolism	0.012853	0.016046	0.012853	0.012853	0.01923	0.025574	0.016046	0.012853	0.025574
Lipoate metabolism	0.00487354	0.017141417	0.046886816	-	0.045458365	0.022939249	-	-	-
Lysine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Methionine and cysteine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Mono-unsaturated fatty acid beta-oxidation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
N-Glycan biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.036383497	-	-
N-Glycan Degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Nicotinate and nicotinamide metabolism	-	-	-	-	-	0.038188	0.04752	-	0.038188
Nitrogen metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Nucleotide Sugar Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.007898496	-	-
O-Glycan biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Omega-3 fatty acid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	0.034871019
Omega-6 fatty acid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Parathio degradation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Pentose and Glucuronate Interconversions	0.00487354	0.024787833	0.046886816	-	0.045458365	0.022939249	-	0.048147215	-
Pentose phosphate pathway	0.00487354	0.037475842	0.046886816	-	0.045458365	0.022939249	-	-	-
Phenylalanine metabolism	-	0.031885	-	-	-	-	-	-	-
Phosphatidylinositol phosphate metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Phytanic acid peroxisomal oxidation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Polyunsaturated fatty acid biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Porphyrin metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Propanoate metabolism	0.00487354	0.037307789	0.046886816	-	0.045458365	0.022939249	-	-	-
Prostaglandin formation from arachidonate	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Prostaglandin formation from dihomo gama-linoleic acid	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Proteoglycan biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Purine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.01462062	-	-
Putative anti-Inflammatory metabolites formation from EPA	0.00487354	0.037307789	0.046886816	0.036047391	0.045458365	0.022939249	-	-	0.010419292
Pyrimidine metabolism	0.00487354	0.047222922	0.046886816	-	0.045458365	0.022939249	0.00487354	-	-
Pyruvate Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
R Group Synthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Riboflavin metabolism	-	-	0.010293	-	-	0.010293	-	-	0.010293
ROS Detoxification	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Saturated fatty acids beta-oxidation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Selenoamino acid metabolism	0.00487354	-	0.020166373	-	0.045458365	0.022939249	-	-	-
Sialic acid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Sphingolipid metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Squalene and cholesterol biosynthesis	0.00487354	-	0.026636417	0.017477523	0.045458365	0.022939249	-	0.034282833	-
Starch and Sucrose Metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
TCA cycle	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Trihydroxycoprostanoyl-CoA beta-oxidation	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Tryptophan metabolism	0.00487354	0.020502479	0.046886816	-	0.045458365	0.022939249	-	-	-
Tyrosine metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Ubiquinone Biosynthesis	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Urea cycle/amino group metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Valine, leucine and isoleucine biosynthesis	0.025574	-	-	-	-	0.00013922	-	-	0.00013922
Valine, leucine and isoleucine degradation	0.00487354	-	0.046886816	0.036047391	0.045458365	0.022939249	-	-	-
Vitamin A (retinol) metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.027476683	-	-
Vitamin B1 (thiamin) metabolism	0.00487354	0.037307789	0.046886816	-	0.045458365	0.022939249	-	-	-
Vitamin B12 (cyanocobalamin) metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Vitamin B2 (riboflavin) metabolism	0.00487354	-	0.046886816	-	0.001680531	0.022939249	0.015796992	-	0.00512562
Vitamin B3 (nicotinate and nicotinamide) metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Vitamin B5 - CoA biosynthesis from pantothenate	0.00487354	-	0.046886816	-	0.045458365	0.022939249	0.015796992	-	-
Vitamin B6 (pyridoxine) metabolism	0.00487354	-	0.020166373	-	0.045458365	0.022939249	-	-	-
Vitamin B9 (folate) metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Vitamin D	0.00487354	-	0.046886816	0.01730947	0.045458365	0.022939249	-	-	-
Vitamin D3 (cholecalciferol) metabolism	0.00487354	-	0.046886816	0.001176372	0.045458365	0.022939249	-	-	-
Vitamin E metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	0.008654735
Vitamin H (biotin) metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Vitamin K metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-
Xenobiotics metabolism	0.00487354	-	0.046886816	-	0.045458365	0.022939249	-	-	-