Genetic upregulation of activated protein C mitigates delayed effects of acute radiation exposure in the mouse plasma

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LC gradient and MS instrument parameters

Untargeted metabolomics

For untargeted 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), 100% isopropanol with 0.1% formic acid (solvent C). Each sample injection was run for 13 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 – 98% A, 2% B till 0.5 minutes; 4.0 minutes – 40% A, 60% B; 8.0 minutes – 2% A, 98% B till 9.0 minutes; 9.5 minutes – 11.8% B, 88.2% C till 11 minutes; 11.5 minutes - 50% A, 50% B, 12.0 minutes – 98% A, 2% B till 13 minutes. Positive mode had a capillary voltage of 2.75 kV, a sampling cone voltage of 30 V, and a source offset of 80 V. Negative mode had a capillary voltage of 2.75 kV, a sampling cone voltage of 20 V, and a source offset of 80 V. The desolvation gas flow was 600 L/h. and the temperature was set to 500 °C. The cone gas flow was 25 L/h, and the source temperature was 100 °C. The data were acquired in the sensitivity MS Mode with a scan time of 1.000 seconds, and inter-scan delay at 0.014 seconds. Real-time mass correction was applied using a solution of Leucine-Enkephalin (1.0 ng/ml) [M+H]+ (m/z 556.2771), [M−H] (m/z 554.2615) in 500 ml of a mixture containing acetonitrile: water (50:50) and 250 µL formic acid at an infusion rate of 20 µL/min utilizing the Waters Lockspray® interface. 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 (Supplementary Figure 3 and 4).

Targeted metabolomics

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 starting with 100% of solvent A and hold for 2.1 minutes and moving to 5% of solvent A over a time period of 12 minute and hold for 1 minute and equilibrating to initial conditions over a time period of 7 minutes using auto sampler temperature 15 °C and oven temperature 30 °C. 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.

Targeted Lipidolomics

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, initial gradient conditions started with 100% of solvent A, shifting towards 99.9% of solvent A over a duration of 3 minutes, 94% of solvent A over a time period of 3 minutes and 25% of solvent A over a period of 4 minutes. Finally, washing with 100% of B for 6 minutes and equilibrating to initial conditions (100% of solvent A) over a time period of 6 minutes using auto sampler

temperature 15 °C and oven temperature 35 °C. 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.

Data processing and statistical analysis

The quality and reproducibility of LC-MS data was ensured using several measures. The column was conditioned using a pooled QC sample that was prepared as a pooled aliquot of all samples in the study set. The QC sample was injected periodically (after every 10 sample injections) to monitor shifts in signal intensities and retention time as measures of reproducibility and ensure high quality data acquisition. A solvent blank sample was also run periodically to monitor and minimize the sample-to-sample carry-over. For targeted data, the detected metabolites were filtered using a signal/noise ratio >20:1 and retention time (RT) tolerance of 5 seconds criteria, to identify the reliable features. The details on LC gradient and mass spectrometry instrument parameters have been provided in the Supplementary information. Data pre-processing include normalization of the raw LC-MS data initially using internal standards. The detected metabolites/features (m/z_rt pairs) with more than 20% missing value were filtered out and 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 variance (CV) were also filtered out. The remaining high-quality features were normalized by Quality Control-Robust LOESS Signal Correction (QC-RLSC) followed by statistical analyses using R (version 4.0.1). For the 67 samples in the study set, the level of differential expression for each metabolite was calculated using an unpaired t-test, comparing sham versus irradiated plasma samples, constrained by p-value<0.05. We also compared gender and genotype based metabolic differences post irradiation in mice plasma. The identities of significantly dysregulated metabolites were confirmed using tandem mass spectrometry. Raw files from untargeted data were converted into MSP format with an in-house developed R package “msmsr” (Li et al., unpublished) and the NIST 2017 MS/MS spectra database. Mummichog v2.0, a Python package specifically designed for untargeted metabolomics was used for pathway analysis [12]. Mummichog v2.0 tests pathway enrichment patterns using permutations and computes the probability for involvement in each pathway. Figures were created using R and BioRender (www.BioRender.com).

Supplementary Table S1. Tandem MS validations for dysregulated metabolites in mice plasma

file_name	precursor_mz/r_rt	Mode	Name	Synonyms	Class	Adduct	Level	CID
20200127_ue1_ppc_plasma_metabolomics_MSMS_NEG_02501.CDF	313.0637_0.84	Negative	Salicylic acid β-D-glucuronide	Salicylglucuronide		[M-H]-	B	313.06, 312.17, 295.22, 1859.01, 183.03, 179.08, 175.03, 137.02, 133.09, 129.06, 117.06, 99.01
20200127_ue1_ppc_plasma_metabolomics_MSMS_NEG_03201.CDF	327.2307_7.71	Negative	1-(12-Octadecanoyl)-2-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphoethanolamine	PE(P-18:0/22:6)	Lipid-PE	[M-H-C37H63O5]-	B	328.23, 327.23, 326.19, 327.18, 309.20, 283.24, 229.19, 191.17, 183.01, 177.16
20200127_ue1_ppc_plasma_metabolomics_MSMS_NEG_05701.CDF	124.0034_0.69	Negative	Taurine	Taurine		[M-H]-	B	124.01, 106.98, 64.9705, 79.96
20200127_ue1_ppc_plasma_metabolomics_MSMS_NEG_08001.CDF	728.557_10.73	Negative	1-(12-Octadecanoyl)-2-(6Z-octadecenoyl)-sn-glycero-3-phosphoethanolamine	PE(P-18:0/18:1)	Lipid-PE	[M-H]-	B	731.56, 730.56, 729.57, 728.56, 446.33, 465.30, 460.27, 447.29, 283.24, 282.25, 281.25, 267.23, 196.03, 140.00
20200127_ue1_ppc_plasma_metabolomics_MSMS_NEG_09601.CDF	850.56_10.13	Negative	1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine	PC(18:0/PC(16:0/22:6)	Lipid-PC	[M+HCO2]-	A	850.56, 790.54, 552.33, 480.31, 327.23, 283.24, 255.23
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_00901.CDF	120.0807_1.14	Positive	N-Acetyl-L-phenylalanine	N-Ac-Phe	Amino acid conjugate	[M+H-C9H9O3]+	B	121.08, 120.08, 119.07, 118.01, 103.05, 93.07, 91.05, 79.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_01001.CDF	121.0282_5.41	Positive	4-Hydroxybenzoic acid	4-OH BnCOOH		[M+H-H2O]+	A	122.09, 111.04, 105.06, 95.04
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_01101.CDF	121.0283_4.46	Positive	5-Methyl-5,6-Dihydrouracil	5,6-Dihydrothymine	Nitrogeneous base	[M+H]+	C	129.06, 69.02
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_01401.CDF	132.0663_0.82	Positive	N-Acetyl-L-alanine	N-Ac-L-alanine	Amino acid conjugate	[M+H]+	A	132.07, 90.05, 86.09
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_02101.CDF	140.0681_0.64	Positive	N-Carboxyethyl-γ-aminobutanic acid	Spermidic acid	Amino acid conjugate	[M+H-2H2O]+	C	140.06, 116.97, 98.96, 98.06, 70.00
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_02501.CDF	144.0805_2.01	Positive	3-(2-Hydroxyethyl)indole	1H-Indole-3-ethanol		[M+H-H2O]+	A	144.08, 143.07, 142.06, 128.05, 127.05, 118.06, 117.06, 115.05, 103.05, 91.05, 77.03
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_03301.CDF	159.091_2.01	Positive	4-(1-Piperazinyl)-1H-indole1	4-(Piperazino)indole		[M+H-C3H5N]+	B	159.09, 157.03, 144.06, 142.06, 133.06, 132.06, 130.06, 117.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_03601.CDF	162.1125_0.67	Positive	L-Carnitine	L-Carnitine	Carnitine	[M+H]+	A	162.11, 103.04, 102.09, 60.08
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_03901.CDF	170.0597_2.01	Positive	DL-Indole-3-lactic acid	3-Indolyllactic acid		[M+H-2H2O]+	A	170.06, 142.06, 115.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_04301.CDF	188.0706_2.01	Positive	L-Tryptophan	Tyr	Amino acid	[M+H-NH3]+	A	188.07, 170.06, 146.06, 118.06
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_04401.CDF	190.0857_2.78	Positive	1H-Indole-3-propanoic acid	3-Indolepropionic acid	potent neuroprotective antioxidant	[M+H]+	A	190.08, 188.07, 172.07, 130.06
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_04501.CDF	203.0528_0.64	Positive	DL-Indole-3-lactic acid	3-Indolyllactic acid		[M+H]+	A	206.08, 188.07, 170.06, 160.07, 146.06, 144.08, 132.08, 130.06, 118.06
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_05901.CDF	261.2205_7.37	Positive	Pinolenic acid	Pinolenic acid	FFA	[M+H-H2O]+	C	261.21, 243.20, 217.19, 135.11, 109.11, 105.07, 81.07
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_06901.CDF	277.215_5.83	Positive	9S-Hydroxy-10E,12Z,15Z-octadecatrienoic acid	9(S)-HOTrE	FFA	[M+H-H2O]+	C	277.18, 221.01, 109.10, 95.08, 81.07, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_07001.CDF	277.2195_6.96	Positive	Stearidonic acid	Moroctic acid C18:4	FFA	[M+H]+	C	277.216, 235.17, 133.10, 125.00, 123.11, 109.10, 107.08, 97.10, 95.08, 81.07, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_07201.CDF	279.2312_7.37	Positive	Pinolenic acid	Pinolenic acid	FFA	[M+H]+	B	279.23, 135.11, 133.10, 131.08, 123.11, 121.10, 119.05, 117.02, 95.08, 81.07, 79.05, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_07501.CDF	281.2471_7.84	Positive	10E,12Z-octadecadienoic acid	Conjugated linoleic acid (10E,12Z)	FFA	[M+H]+	B	281.14, 263.23, 245.22, 221.02, 123.11, 121.10, 119.08, 111.11, 109.10, 97.10, 95.08, 93.07
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_07901.CDF	283.2631_8.35	Positive	trans-Vaccenic acid	(11E)-11-Octadecenoic acid	FFA	[M+H]+	B	265.25, 247.24, 209.18, 129.06, 125.00, 123.11, 121.10, 111.10, 109.10, 107.08, 93.07, 83.08, 81.06, 71.08, 69.07, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_08301.CDF	288.2527_4.79	Positive	Lauric acid diethanolamide	Alkamide LE		[M+H]+	C	288.25, 270.24, 109.10, 106.09, 95.08, 88.08, 81.07, 71.08, 60.04
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_08601.CDF	305.2479_7.72	Positive	cis-5,8,11,14-Eicosatetraenoic acid	Arachidonic acid	FFA	[M+H]+	A	305.24, 304.23, 269.22, 259.20, 245.22, 221.15, 199.15, 193.12, 191.18, 189.13, 122.10, 120.09, 118.07, 109.10, 107.08
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_09601.CDF	307.2631_8.06	Positive	5Z,11Z,14Z-Eicosatrienoic acid	5,6-EpETrE	FFA	[M+H]+	B	307.26, 289.25, 271.24, 123.12, 109.10, 81.07, 79.05, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_10101.CDF	319.2638_8.65	Positive	ω-3 Arachidonic acid methyl ester	ω-3 Arachidonic acid methyl ester		[M+H]+	B	319.15, 287.23, 161.13, 147.12, 123.11, 121.10, 119.08, 117.07 107.08, 97.10, 95.08, 93.07, 91.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_10701.CDF	325.2111_7.86	Positive	Marevin 1	Marevin 1		[M+H-2H2O]+	A	325.21, 173.13, 171.11, 145.10, 145.10, 143.08, 141.07, 131.08, 129.07, 121.10, 119.08, 117.07, 95.08, 93.07,91.06, 81.07,79.05, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_10901.CDF	327.2322_7.25	Positive	10-hydroxy-4Z,7Z,11E,13Z,16Z,19Z-docosahexaenoic acid	(n)10-HDoHE	FFA	[M+H-H2O]+	A	327.23, 273.18, 267.21, 265.19, 259.17, 163.14, 59.11, 155.08, 149.13, 145.10, 143.10, 141.07, 139.07,123.11, 119.08, 105.07,95.08, 93.07,81.07 ,79.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_11001.CDF	329.2086_4.29	Positive	5α-Dihydrocortisol	Hydrotasone	Cortisol Metabolite	[M+H-2H2O]+	B	329.21, 311.24, 283.20, 171.11, 169.10, 149.13, 145.10, 143.08, 141.08, 131.08, 119.08, 117.07, 95.08, 91.04, 81.07, 79.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_11101.CDF	329.2481_7.61	Positive	cis-5,8,11-Eicosatrienoic acid	cis-5,8,11-Eicosatrienoic acid	FFA	[M+Na]+	A	330.25, 329.25, 311.24, 293.23, 283.20, 260.22, 259.17, 201.16, 199.14, 197.12, 190.12, 187.11, 185.13, 185.13, 181.10, 179.11, 123.12, 121.10, 119.08, 109.10, 95.08, 93.07, 91.04, 81.07, 79.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_12001.CDF	357.2798_5.57	Positive	Chenodeoxycholic acid	chenocholic acid	Bile Acid	[M+H-2H2O]+	A	357.27, 147.12, 145.10, 135.12, 123.11, 121.10, 119.08, 109.10, 107.08, 101.06, 97.10, 95.06, 93.07, 81.07, 79.05, 77.03
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_14301.CDF	365.3182_7.28	Positive	7α,24(S)-Dihydroxycholesterol	7α,24(S)-Dihydroxycholesterol	Oxysterol	[M+H-2H2O]+	A	365.25, 309.28, 299.19, 217.19, 203.18, 201.16, 191.17, 187.14, 149.13, 147.12, 135.11, 123.11, 121110, 119.08, 109.10, 107.08, 105.07, 95.08, 81.07
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_14701.CDF	369.3512_10.89	Positive	5α-Cholest-7-en-3β-ol	Lathosterol		[M+H-H2O]+	A	369.35, 368.34, 287.27, 259.24, 243.21, 215.18, 163.15, 161.13, 149.13, 147.12, 145.10, 135.12, 123.11, 109.10, 95.08, 93.07, 71.08, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_14801.CDF	369.3518_10.2	Positive	5α-Cholest-7-en-3β-ol	Lathosterol		[M+H-H2O]+	A	
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_14901.CDF	370.2712_7.6	Positive	N-Arachidonylmalonimide	N-Arachidonylmalonimide	Monoacylglycerol lipase (MAGL) inhibitor	[M+H]+	C	370.28, 328.22, 189.16, 161.13, 151.15, 135.11, 121.10, 83.07,81.07, 79.05, 69.05, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_15101.CDF	370.2949_5.1	Positive	N-Oleoyl-L-serine	N-Oleoyl-L-serine	Amino acid conjugate	[M+H]+	B	370.28, 149.13, 135.12, 123.11, 121.10, 97.10, 95.08, 93.07, 81.07, 79.05, 71.08, 67.05
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_16201.CDF	380.2516_5.58	Positive	D-erythro-Sphingosine-1-phosphate	S1P	Lipid	[M+H]+	B	380.28, 362.25, 264.27
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_16301.CDF	380.2846_7.99	Positive	Prostaglandin E1 ethanolamide	Alprostadil	Prostaglandin	[M+H-H2O]+	C	380.28, 229.19, 181.16, 156.01, 149.13, 131.00, 15.06
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_17401.CDF	393.2992_12.45	Positive	Bis(2-ethylhexyl) adipate	DEHA		[M+Na]+	C	393.29, 281.17
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_18201.CDF	400.3417_5.79	Positive	Palmitoylcarnitine	Palmitoylcarnitine	Carnitine	[M+H]+	B	400.33, 341.26, 144.09, 85.03
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_22501.CDF	468.3085_5.62	Positive	1-Myristoyl-sn-glycero-3-phosphocholine	LPC(14:0)	LPC	[M+H]+	A	469.30, 468.30, 450.30, 285.24, 258.12, 184.07, 166.06, 163.00, 125.00, 104.11, 86.10
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_23201.CDF	496.3402_6.36	Positive	1-Palmitoyl-sn-glycero-3-phosphocholine	LPC(16:0)	LPC	[M+H]+	A	497.34, 496.34, 478.33, 419.25, 313.27, 258.11, 184.07, 166.06, 163.02, 125.00, 104.11, 86.10, 60.08
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_23301.CDF	508.3752_6.77	Positive	1-(12-Octadecanyl)-sn-glycero-3-phosphocholine	LPC(P-18:0)	LPC	[M+H]+	A	508.39, 449.25, 240.13, 184.07, 181.02, 166.06, 136.99, 125.00, 111.07, 104.11, 98.9286 ,91, 86.10, 83.08
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_23501.CDF	510.3902_7.41	Positive	1-O-Octadecyl-sn-glyceryl-3-phosphorylcholine	LPC(O-18:0)	LPC	[M+H]+	A	510.36, 327.28, 240.09, 184.07, 166.06, 125.00, 104.11, 86.10, 60.08
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_23701.CDF	524.3715_7.15	Positive	1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine	LPC(18:0)	LPC	[M+H]+	A	524.37, 506.36, 483.36, 447.29, 341.31, 258.11, 184.07, 125.00, 104.11, 86.10, 60.08
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_24001.CDF	532.3735_7.36	Positive	1-O-Octadecyl-sn-glycerol-3-phosphorylcholine	LPC(O-18:0)	LPC	[M+H]+	A	532.27, 473.26, 429.24, 398.17, 183.09, 146.98, 104.11, 86.10, 71.09
20200124_ue1_ppc_plasma_metabolomics_MSMS_POS_24601.CDF	572.3697_6.61	Positive	1-O-Hexadecyl-2-O-(2E-butenoyl)-sn-glyceryl-3-phosphocholine	Butenoyl PAF	Potent phospholipid activator	[M+Na]+	A	574.38, 572.37, 572.37, 552.30, 514.29, 515.31, 513.29, 367.31, 184.07, 146.98

Supplementary Table S2. List of dysregulated metabolites following exposure to 9.5 Gy of gamma-radiation, 6 months' post irradiation

| | | | Wild Type | | |

Supplementary Table S3. List of dysregulated metabolites and lipids upon exposure to 9.5 Gy of gamma radiation, 6 months' post irradiation

		Wild Type										APCHI																							
		Overall				Male						Male				Female						Female				Wild Type				APCHI			
Mode	Name	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*	*p-value*	*FDR*	*Fold Change*	*Log2(FC)*
Metabolomics	Phosphorylcholine	0.14498	0.73	0.89963	-0.1526	0.02456	0.94	0.71276	-0.4885	0.90032	1	0.98504	-0.0217	0.39624	0.98	0.89198	-0.1649	0.62441	0.99	1.1016	0.1396	0.01521	0.65	0.78912	-0.3417	0.78527	1	1.0446	0.063	0.07037	0.81	0.82543	-0.2768	0.90367	1	0.98278	-0.0251
Metabolomics	Citric Acid	0.01858	0.3	1.4932	0.57941	0.03004	0.94	1.7505	0.8078	0.30341	0.9	1.5786	0.65867	0.30363	0.98	1.5724	0.65297	0.79993	0.99	0.90841	-0.1386	0.0123	0.65	1.7591	0.81481	0.62737	1	1.135	0.18271	0.03747	0.68	1.7626	0.81767	0.34738	1	1.1839	0.2435
Metabolomics	Glycerophosphocholine	0.07828	0.73	0.77966	-0.3591	0.03602	0.94	0.57587	-0.7962	0.60849	0.96	0.89831	-0.1547	0.3571	0.98	0.75023	-0.4146	0.98612	0.99	1.0418	0.05905	0.02171	0.65	0.64804	-0.6258	0.71201	1	0.97116	-0.0422	0.06672	0.81	0.70912	-0.4959	0.51723	1	0.85842	-0.2203
Metabolomics	Xanthylic Acid	0.02209	0.32	1.3382	0.42026	0.03997	0.94	1.5047	0.5895	0.62303	0.96	1.3874	0.47244	0.62187	0.98	1.1413	0.19067	0.26394	0.99	1.3465	0.42925	0.07213	0.73	1.2652	0.33932	0.2687	1	1.3199	0.39604	0.03911	0.68	1.4884	0.5738	0.28466	1	1.2109	0.27614
Metabolomics	Hypoxanthine	0.44045	0.85	1.0732	0.10194	0.46144	0.96	1.0455	0.06329	0.96841	1	0.85225	-0.2307	0.15148	0.98	0.7507	-0.4153	0.57552	0.99	1.3144	0.39434	0.55501	0.92	1.0517	0.07295	0.11461	0.85	1.2319	0.3009	0.7177	1	1.9302	0.95	0.41044	1	1.1806	0.23956
Metabolomics	4-Aminobenzoic Acid	0.27074	0.73	1.2314	0.30028	0.04436	0.94	1.5912	0.6701	0.15419	0.93	0.49607	-0.1014	0.16975	0.98	1.6781	0.74682	0.29507	0.99	0.81426	-0.2964	0.0126	0.65	1.6362	0.71035	0.16705	1	0.74086	-0.4337	0.39468	0.85	1.2854	0.36218	0.50275	1	1.1806	0.23956
Metabolomics	N-Acetylornithine	1E-04	0.01	0.61953	-0.6908	0.04687	0.94	0.70607	-0.5021	0.80506	0.48	0.32702	-1.6126	0.70591	1	0.9337	-0.099	0.15487	0.99	0.62912	-0.6686	0.06349	0.68	0.80001	-0.3219	0.00844	0.04	0.50278	-0.992	0.00031	0.03	0.50712	-0.9796	0.08401	1	0.74961	-0.4158
Metabolomics	Citrulline Reduced	0.23477	0.73	1.062	0.08676	0.68087	0.94	0.67196	-0.5875	0.40037	0.93	1.1468	0.19482	0.48	0.98	0.7887	-0.3425	0.54257	0.99	1.0685	0.09552	0.59502	0.94	1.0336	0.04575	0.60158	1	1.0798	0.11497	0.66188	0.81	1.2756	0.35121	0.72712	1	0.90817	-0.139
Metabolomics	Methylthioadenosine	0.13261	0.73	0.93995	-0.0893	0.05104	0.94	0.57384	-0.8013	0.49576	0.94	1.3829	0.46771	0.24394	0.98	0.94601	-0.0801	0.30585	0.99	1.3697	0.45383	0.01895	0.65	0.72423	-0.4655	0.23966	1	1.3274	0.40857	0.12583	0.85	0.78988	-0.3403	0.59126	1	1.0937	0.12924
Metabolomics	Arginine	6.6E-05	0.01	0.61579	-0.6095	0.05125	0.94	0.71571	-0.4484	0.80424	0.48	0.32615	-1.6164	0.50424	0.98	0.80691	-0.157	0.04151	0.99	0.63944	-0.6451	0.04438	0.65	0.79002	-0.34	0.00046	0.04	0.50761	-0.9782	0.00001	0.03	0.50443	-0.9873	0.06296	1	0.74272	-0.4291
Metabolomics	Glycine	0.10109	0.73	1.1092	0.14953	0.07577	0.94	1.2571	0.33014	0.11005	0.92	1.2271	0.29514	0.11605	0.98	1.197	0.25463	0.12606	0.98	0.8696	-0.2016	0.01864	0.65	1.2174	0.28274	0.02718	0.81	1.1864	0.24662	0.68651	1	1.2034	0.26853	0.14	0.99	0.98	0
Metabolomics	Dopamine	0.5142	0.89	1.1844	0.2441	0.14861	0.94	1.3031	0.3819	0.16153	0.93	1.4517	0.53771	0.34705	0.98	0.9285	-0.107	0.81016	0.99	1.0614	0.08598	0.75664	0.95	1.1859	0.24602	0.39613	1	1.187	0.2469	0.03807	0.68	1.3506	0.43362	0.46411	1	0.99623	-0.0054
Metabolomics	Proline	0.009	0.25	0.80794	-0.3077	0.17569	0.94	0.82894	-0.2691	0.40051	0.93	0.81513	-0.2949	0.17996	0.98	0.81199	-0.2865	0.62146	0.99	0.95392	-0.0681	0.04214	0.65	0.81873	-0.2885	0.20236	1	0.83864	-0.2539	0.03025	0.68	0.74313	-0.4283	0.16029	1	0.88471	-0.1767
Metabolomics	Glycine	0.01563	0.27	0.7709	-0.4798	0.02886	0.94	0.80185	-0.3186	0.71903	0.97	0.90142	-0.1508	0.40402	0.98	0.85118	-0.2351	0.62868	0.99	0.84102	-0.2498	0.04398	0.65	0.81708	-0.2915	0.12464	1	0.83126	-0.2634	0.06126	0.81	0.63568	-0.6536	0.107	1	0.68442	-0.2421
Metabolomics	Xanthurenic Acid	0.00713	0.25	0.72704	-0.4599	0.2105	0.94	0.69168	-0.5318	0.20239	0.93	0.66414	-0.5904	0.06149	0.98	0.72435	-0.4652	0.89646	0.99	0.99431	-0.0082	0.02841	0.65	0.70492	-0.5045	0.19666	1	0.77992	-0.3586	0.02697	0.68	0.63368	-0.6582	0.14256	1	0.84674	-0.24
Metabolomics	Indoleacrylic Acid	0.00751	0.25	0.7711	-0.375	0.23268	0.94	0.77796	-0.3622	0.17543	0.93	0.69214	-0.5309	0.04996	0.98	0.73696	-0.4404	0.97952	0.99	1.0149	0.02129	0.02597	0.65	0.75765	-0.4004	0.22361	1	0.82081	-0.2849	0.02396	0.68	0.6906	-0.5341	0.16772	1	0.86797	-0.2043
Metabolomics	Tryptophan	0.01077	0.25	0.72132	-0.4715	0.29173	0.94	0.67739	-0.4564	0.17647	0.93	0.64609	-0.6437	0.04973	0.98	0.66409	-0.6437	0.45973	0.98	0.67167	-0.5742	0.02534	0.65	0.72026	-0.4756	0.03407	0.65	0.70386	-0.5066	0.02455	0.68	0.6227	-0.6735	0.19268	1	0.83576	-0.2557
Metabolomics	Indole	0.00809	0.25	0.74813	-0.4186	0.31663	0.94	0.79754	-0.3264	0.19559	0.93	0.6773	-0.5621	0.05173	0.98	0.70319	-0.508	0.9068	0.99	0.99909	-0.0013	0.03456	0.65	0.74688	-0.4211	0.19151	1	0.78937	-0.3412	0.0339	0.68	0.67273	-0.5719	0.13008	1	0.83963	-0.2522
Metabolomics	N-Acetylornithine	0.01357	0.26	0.79368	-0.3963	0.3354	0.94	0.71061	-0.4929	0.19368	0.93	0.48755	-0.1364	0.93292	1	1.1561	0.20683	0.1201	0.99	0.71649	-0.3833	0.4014	0.89	0.88615	-0.1744	0.00763	0.45	0.5674	-0.6273	0.02433	0.68	0.60196	-0.7323	0.2633	1	0.93977	-0.0896
Metabolomics	4-Aminobenzoic Acid	0.01052	0.25	0.86395	-0.2311	0.87863	0.988	1.0261	0.03746	0.05787	0.93	0.74687	-0.2903	0.56107	0.98	0.80077	-0.3205	0.46874	0.99	0.90614	-0.1418	0.14964	0.89	0.80426	-0.3158	0.10291	1	0.85025	-0.2349	0.01297	0.68	0.87694	-0.1894	0.03336	1	0.85203	-0.2349
Lipidomics	LPC(22:0)	0.30446	0.49	0.87237	-0.197	0.00145	0.107	0.72071	-0.4725	0.45007	0.68	1.0947	0.13056	0.42195	0.86	0.8101	-0.3038	0.52384	0.74	0.92206	-0.1171	0.01002	0.07	0.75561	-0.4043	0.81024	0.89	0.98395	-0.0233	0.54777	0.8	0.89582	-0.1587	0.41847	0.68	0.84944	-0.2354
Lipidomics	PE(O-18:0/22:4)	0.3515	0.54	0.89624	-0.158	0.00264	0.107	0.59375	-0.7528	0.47678	0.71	1.0853	0.11806	0.09528	0.61	1.3327	0.41435	0.16944	0.47	0.82803	-0.2845	0.34357	0.48	0.84535	-0.2424	0.41108	0.59	0.90842	-0.1386	0.09179	0.18	0.7574	-0.4009	0.48608	0.7	0.1097	0.1107
Lipidomics	PC(16:0/18:2)	0.01648	0.06	0.80962	-0.3045	0.00062	0.107	0.69841	-0.5179	0.06896	0.28	0.97242	-0.0396	0.94192	0.98	0.78409	-0.3509	0.00563	0.07	0.76887	-0.3802	0.00553	0.05	0.73755	-0.4355	0.00149	0.07	0.72521	-0.4624	0.01188	0.16	0.78274	-0.3534	0.1606	0.52	0.79225	-0.3917
Lipidomics	LPC(20:0)	0.90655	0.95	0.88683	-0.1733	0.00316	0.107	0.72191	-0.4701	0.78224	0.91	0.9428	-0.085	0.93777	0.98	0.85584	-0.2246	0.29553	0.58	0.70037	-0.5138	0.14414	0.28	0.7778	-0.3622	0.25594	0.43	0.79571	-0.3297	0.70843	0.86	0.95667	-0.0639	0.64436	0.82	0.81703	-0.2915
Lipidomics	PC(17:0/18:2)	0.00039	0.01	0.78459	-0.35	0.00325	0.107	0.7348	-0.4446	0.12453	0.38	0.74136	-0.4318	0.19133	0.73	0.84291	-0.2466	0.01846	0.36	0.77587	-0.3661	0.00168	0.04	0.78214	-0.3545	0.00339	0.04	0.73332	-0.4475	0.00247	0.07	0.75922	-0.3974	0.03587	0.4	0.8	-0.2969
Lipidomics	PC(17:0/22:6)	0.01	0.05	0.7022	-0.5124	0.19003	0.107	0.7662	-0.3842	0.30093	0.56	0.84319	-0.2461	0.39905	0.86	0.90137	-0.1498	0.12473	0.43	0.82788	-0.2705	0.00603	0.05	0.83803	-0.2515	0.04582	0.18	0.83409	-0.2603	0.04586	0.18	0.83497	-0.2602	0.1136	0.49	0.8678	-0.2046
Lipidomics	PI 16_0:20_1	0.00027	0.01	0.78557	-0.3482	0.00454	0.107	0.73527	-0.4436	0.00193	0.11	0.62605	-0.6757	0.18336	0.73	0.8356	-0.2591	0.22837	0.51	0.83499	-0.2602	0.02009	0.04	0.78129	-0.3561	0.00361	0.04	0.74278	-0.429	0.00057	0.03	0.7414	-0.4317	0.08967	0.45	0.83532	-0.2596
Lipidomics	PE(O-18:0/18:1)	0.01567	0.06	0.77597	-0.3659	0.00534	0.107	0.62561	-0.6767	0.3754	0.63	0.84319	-0.2461	0.79048	0.92	0.88835	-0.1547	0.10103	0.42	0.7326	-0.4489	0.0238	0.11	0.73703	-0.4402	0.03435	0.11	0.76185	-0.3924	0.02766	0.14	0.73622	-0.4418	0.20647	0.53	0.82461	-0.2782
Lipidomics	PC(18:0/18:3)	2.8E-06	0	0.86757	-0.2531	0.00543	0.107	0.56846	-0.8148	0.00372	0.13	0.55583	-0.8475	0.00168	0.19	0.66939	-0.5802	0.00168	0.15	0.69934	-0.5175	0.00064	0.04	0.62624	-0.6768	0.00054	0.04	0.58157	-0.8576	0.00008	0.01	0.50074	-0.9994	0.00184	0.16	0.65121	-0.6166
Lipidomics	PE(18:2/16:1)	0.00319	0.03	0.74147	-0.4315	0.00678	0.107	0.66429	-0.5901	0.02754	0.2	0.62156	-0.686	0.30507	0.82	0.81931	-0.2875	0.14568	0.46	0.76825	-0.3804	0.00806	0.07	0.73389	-0.4464	0.00611	0.04	0.66824	-0.5816	0.00351	0.07	0.69772	-0.5193	0.13502	0.49	0.7986	-0.3245
Lipidomics	PC(20:0/22:6)	0.10882	0.24	0.75117	-0.4128	0.0068	0.107	0.64557	-0.6314	0.89268	0.96	0.94225	-0.0858	0.20592	0.73	0.69821	-0.5183	0.0941	0.42	0.63191	-0.6622	0.00419	0.05	0.66999	-0.5778	0.08764	0.2	0.74331	-0.428	0.02823	0.14	0.82626	-0.2753	0.12451	0.49	0.67628	-0.5643
Lipidomics	PC(16:0/22:5)	0.22414	0.41	0.81062	-0.3028	0.00686	0.107	0.70232	-0.5098	0.68251	0.94	0.92431	-0.1115	0.42349	0.86	0.71838	-0.4353	0.08338	0.66	0.82618	-0.2688	0.69421	0.85	0.71045	-0.4932	0.14162	0.37	0.72521	-0.4624	0.01188	0.16	0.87925	-0.1857	0.2661	0.53	0.74296	-0.4426
Lipidomics	PC(16:0/22:6)	0.06477	0.17	0.8359	-0.2586	0.00689	0.107	0.73346	-0.4472	0.61104	0.83	0.92701	-0.1093	0.17979	0.73	0.79862	-0.3244	0.17644	0.47	0.80509	-0.3128	0.03059	0.05	0.76463	-0.3872	0.1243	0.25	0.85394	-0.2278	0.32729	0.6	0.86975	-0.2013	0.11628	0.49	0.8012	-0.3198
Lipidomics	LPC(18:2)	0.13568	0.28	0.9186	-0.1225	0.00692	0.107	0.80572	-0.3117	0.80658	0.91	0.96052	-0.0581	0.70364	0.91	0.9424	-0.0856	0.78565	0.9	0.98934	-0.0155	0.02318	0.11	0.8622	-0.2139	0.48842	0.64	0.95369	-0.0684	0.06095	0.21	0.87854	-0.1868	0.70921	0.86	0.96229	-0.0555
Lipidomics	PE(O-18:0/18:2)	0.00038	0.01	0.66756	-0.583	0.00279	0.107	0.62139	-0.6864	0.01606	0.16	0.63893	-0.6563	0.11126	0.49	0.67924	-0.5558	0.09954	0.32	0.57258	-0.8044	0.00171	0.04	0.60313	-0.7312	0.00063	0.04	0.54637	-0.875	0.02639	0.14	0.69386	-0.5273	0.61461	0.91	0.63789	-0.6484
Lipidomics	PA 18_1:20_3	0.00452	0.03	0.82431	-0.2787	0.00769	0.107	0.74857	-0.4178	0.03204	0.21	0.73504	-0.4441	0.1903	0.73	0.85084	-0.2331	0.59077	0.77	0.89933	-0.1531	0.03328	0.05	0.79531	-0.3304	0.07018	0.17	0.82033	-0.2857	0.03661	0.07	0.7817	-0.3553	0.24283	0.55	0.87238	-0.197
Lipidomics	PE(O-18:0/22:6)	0.00069	0.01	0.76321	-0.3899	0.00868	0.107	0.68731	-0.541	0.3031	0.56	0.82319	-0.2807	0.20195	0.73	0.79154	-0.3373	0.0957	0.42	0.73126	-0.4489	0.0238	0.11	0.73153	-0.451	0.02607	0.09	0.77571	-0.3664	0.03049	0.08	0.74171	-0.4311	0.04755	0.41	0.78699	-0.3456
Lipidomics	PE(18:2/20:5)	0.00657	0.04	0.68285	-0.5932	0.00199	0.107	0.62919	-0.6684	0.06938	0.28	0.55012	-0.8605	0.17938	0.73	0.67479	-0.5675	0.10064	0.42	0.54274	-0.8802	0.00384	0.05	0.61515	-0.6719	0.0091	0.06	0.51587	-0.9576	0.03258	0.15	0.69797	-0.5188	0.07484	0.44	0.62486	-0.6784
Lipidomics	PC(20:0/18:2)	0.26027	0.46	0.80566	-0.3118	0.009	0.107	0.73973	-0.4349	0.02508	0.19	0.63643	-0.6519	0.49904	0.89	0.78712	-0.3454	0.07932	0.41	0.5312	-0.9127	0.05002	0.17	0.76599	-0.3846	0.0048	0.04	0.55832	-0.8408	0.6563	0.85	0.88667	-0.1735	0.27806	0.59	0.71497	-0.4841
Lipidomics	PC(15:0/18:1)	0.1421	0.29	0.84313	-0.2462	0.00905	0.107	0.73517	-0.4439	0.28182	0.54	0.78071	-0.3571	0.35634	0.86	0.88031	-0.1896	0.23176	0.54	0.80672	-0.3141	0.01419	0.09	0.78059	-0.3574	0.21834	0.39	0.84039	-0.2509	0.2514	0.51	0.83669	-0.2572	0.36192	0.65	0.85023	-0.2341
Lipidomics	PC(20:0/20:4)	0.27385	0.46	0.79384	-0.3331	0.00911	0.107	0.60047	-0.7354	0.35685	0.57	0.81407	-0.2951	0.56103	0.89	0.78065	-0.3572	0.08533	0.41	0.5776	-0.7919	0.03894	0.14	0.71038	-0.4519	0.02444	0.09	0.61656	-0.6035	0.71261	0.86	0.8614	-0.2119	0.27676	0.59	0.72022	-0.4735
Lipidomics	DAG(18:1/20:5)	9.7E-06	0	0.42857	-1.2224	0.00922	0.107	0.3838	-1.3816	0.02123	0.19	0.3241	-1.6255	0.08484	0.5	0.40735	-1.2957	0.11794	0.43	0.54506	-0.8755	0.00077	0.04	0.40594	-1.3007	0.00346	0.04	0.41428	-1.2713	0.00075	0.03	0.407	-1.2969	0.0042	0.16	0.46111	-1.1168
Lipidomics	DAG(18:2/20:4)	6.2E-06	0	0.41895	-1.2552	0.01157	0.125	0.43496	-1.201	0.22881	0.2	0.25338	-1.9806	0.05098	0.4	0.46841	-1.0942	0.04525	0.4	0.59459	-0.75	0.00108	0.04	0.45861	-1.1247	0.00205	0.03	0.34225	-1.5469	0.00238	0.03	0.36508	-1.4537	0.0058	0.16	0.51641	-0.9534
Lipidomics	PC(16:0/20:4)	0.0471	0.14	0.88118	-0.1828	0.01202	0.125	0.66528	-0.588	0.21881	0.5	0.84008	-0.2517	0.17746	0.73	0.74371	-0.4272	0.02269	0.78	0.92165	-0.1177	0.0548	0.25	0.75068	-0.4092	0.19463	0.47	0.79159	-0.3372	0.2209	0.55	0.81148	-0.3015	0.11428	0.49	0.81147	-0.3015
Lipidomics	LPA 18_2	0.14915	0.3	0.84133	-0.2493	0.01217	0.125	0.71063	-0.4928	0.05137	0.26	0.58004	-0.7858	0.95821	0.98	0.98723	-0.0185	0.83564	0.92	1.0193	0.02759	0.1014	0.23	0.82616	-0.2755	0.22223	0.4	0.78821	-0.3434	0.01809	0.12	0.72655	-0.4609	0.85082	0.95	1.001	0.00138
Lipidomics	PC(18:2/22:5)	0.45057	0.64	0.86024	-0.2172	0.01324	0.126	0.78885	-0.3422	0.91084	0.96	0.84971	-0.235	0.54914	0.89	0.86052	-0.2581	0.70364	0.91	0.9424	-0.0856	0.78565	0.9	0.88934	-0.0155	0.02318	0.11	0.8622	-0.2139	0.48842	0.64	0.95369	-0.0684	0.06095	0.21	0.87854	-0.1868
Lipidomics	PE(O-18:0/18:2)	0.01425	0.06	0.67074	-0.5756	0.00126	0.126	0.65974	-0.6	0.17532	0.63	0.63893	-0.6563	0.11126	0.49	0.67924	-0.5558	0.09954	0.32	0.57258	-0.8044	0.00171	0.04	0.60313	-0.7312	0.00063	0.04	0.54637	-0.875	0.02639	0.14	0.69386	-0.5273	0.61461	0.91	0.63789	-0.6484
Lipidomics	LPC(24:0)	0.30065	0.49	0.91188	-0.1331	0.01392	0.126	0.79054	-0.3391	0.80988	0.91	1.0205	0.02928	0.79314	0.92	0.92645	-0.1102	0.17742	0.47	0.86289	-0.2128	0.0653	0.18	0.84614	-0.241	0.30057	0.49	0.92528	-0.112	0.59136	0.81	0.92382	-0.1143	0.38447	0.67	0.90016	-0.1518
Lipidomics	PC(16:0/16:0)	0.00177	0.02	0.78736	-0.3449	0.01432	0.126	0.74605	-0.4227	0.11661	0.36	0.76315	-0.39	0.14982	0.73	0.77598	-0.3659	0.07771	0.41	0.80085	-0.3204	0.00395	0.05	0.75646	-0.4027	0.00901	0.06	0.77262	-0.3722	0.01497	0.11	0.78838	-0.343	0.04719	0.41	0.78631	-0.3468
Lipidomics	PC(17:0/20:4)	0.00737	0.04	0.82869	-0.2706	0.01517	0.126	0.73318	-0.4478	0.1771	0.48	0.79172	-0.3386	0.06115	0.56	0.77966	-0.3591	0.85291	0.93	1.017	0.02429	0.00351	0.04	0.75508	-0.4053	0.2606	0.47	0.90584	-0.1427	0.61464	0.91	0.78399	-0.3511	0.33947	0.63	0.78836	-0.3465
Lipidomics	PC(18:2/18:2)	0.00646	0.04	0.75493	-0.4056	0.01605	0.133	0.71886	-0.4762	0.01111	0.16	0.57347	-0.8022	0.59415	0.89	0.86735	-0.2053	0.03434	0.4	0.6832	-0.5496	0.02923	0.12	0.78206	-0.3547	0.00074	0.01	0.59858	-0.7404	0.00493	0.08	0.72099	-0.472	0.1722	0.52	0.79663	-0.328
Lipidomics	PC(16:0/20:5)	0.00231	0.02	0.66963	-0.5786	0.01692	0.134	0.62303	-0.6826	0.07688	0.3	0.66364	-0.5915	0.07288	0.58	0.69186	-0.69	0.08931	0.42	0.64442	-0.6339	0.00222	0.04	0.62653	-0.6751	0.00851	0.05	0.64009	-0.6436	0.03069	0.15	0.70704	-0.5001	0.03187	0.4	0.82605	-0.2369
Lipidomics	PE(18:0/18:2)	3.2E-05	0	0.79739	-0.3246	0.01725	0.134	0.65655	-0.6854	0.06507	0.28	0.61955	-0.6908	0.24551	0.84	0.68976	-0.5372	0.05164	0.32	0.7528	-0.4104	0.00246	0.04	0.73667	-0.4357	0.00151	0.05	0.71847	-0.4396	0.00236	0.03	0.73776	-0.4377	0.00134	0.05	0.8188	-0.2897
Lipidomics	PE(18:2/18:2)	0.00623	0.04	0.69336	-0.5283	0.01831	0.135	0.62527	-0.6774	0.07875	0.3	0.62772	-0.6718	0.91282	0.97	0.8396	-0.2522	0.00647	0.28	0.53398	-0.9051	0.08452	0.2	0.71452	-0.485	0.00063	0.01	0.54736	-0.8695	0.03138	0.1	0.67514	-0.5668	0.1058	0.49	0.71576	-0.4824
Lipidomics	PC(18:2/20:1)	0.3871	0.58	0.84936	-0.2356	0.01839	0.135	0.78205	-0.3574	0.02132	0.19	0.58978	-0.7618	0.75578	0.91	0.85124	-0.2324	0.17107	0.47	0.73347	-0.4472	0.01115	0.09	0.81551	-0.2942	0.00693	0.06	0.60815	-0.7175	0.68251	0.85	0.90806	-0.1391	0.4339	0.68	0.85023	-0.2341
Lipidomics	PI 20_0:20_3	0.00126	0.02	0.64144	-0.6343	0.01899	0.135	0.58785	-0.7665	0.02383	0.16	0.51407	-0.9605	0.29154	0.73	0.70124	-0.5133	0.2476	0.52	0.6809	-0.5546	0.00392	0.05	0.63803	-0.6444	0.00349	0.04	0.58108	-0.8459	0.02444	0.09	0.61463	-0.7022	0.08713	0.45	0.60297	-0.5291
Lipidomics	PE(P-18:1/22:6)	0.56956	0.73	0.91786	-0.1237	0.02015	0.139	0.72332	-0.4673	0.27619	0.54	1.1492	0.20069	0.53168	0.89	0.86747	-0.2051	0.48193	0.71	1.0916	0.12641	0.02532	0.11	0.78272	-0.3534	0.25073	0.43	1.0984	0.13544	0.44632	0.73	0.88323	-0.1791	0.96782	0.99	0.95436	-0.0674
Lipidomics	PG 16_0:18_1_2	0.0046	0.03	0.74281	-0.429	0.02069	0.139	0.7163	-0.4814	0.00595	0.13	0.62698	-0.6735	0.02639	0.5	0.69568	-0.5235	0.15778	0.47	0.73347	-0.4472	0.00111	0.04	0.71187	-0.4903	0.00757	0.05	0.67868	-0.5634	0.03212	0.15	0.77305	-0.3734	0.05595	0.41	0.70997	-0.4946
Lipidomics	LPC(22:1)	0.44628	0.69	0.85454	-0.2246	0.02227	0.143	0.84043	-0.214	0.90354	0.96	0.99033	-0.0142	0.60019	0.93	0.88214	-0.1809	0.20001	0.53	0.72065	-0.4726	0.12201	0.25	0.83488	-0.2404	0.2224	0.42	0.72704	-0.4576	0.59781	0.81	1.011	0.01571	0.50165	0.71	0.83173	-0.2659
Lipidomics	LPC(18:0)	0.65251	0.79	0.99201	-0.0116	0.02239	0.143	0.82334	-0.2805	0.02685	0.2	1.307	0.38625	0.88345	0.95	0.99148	-0.0124