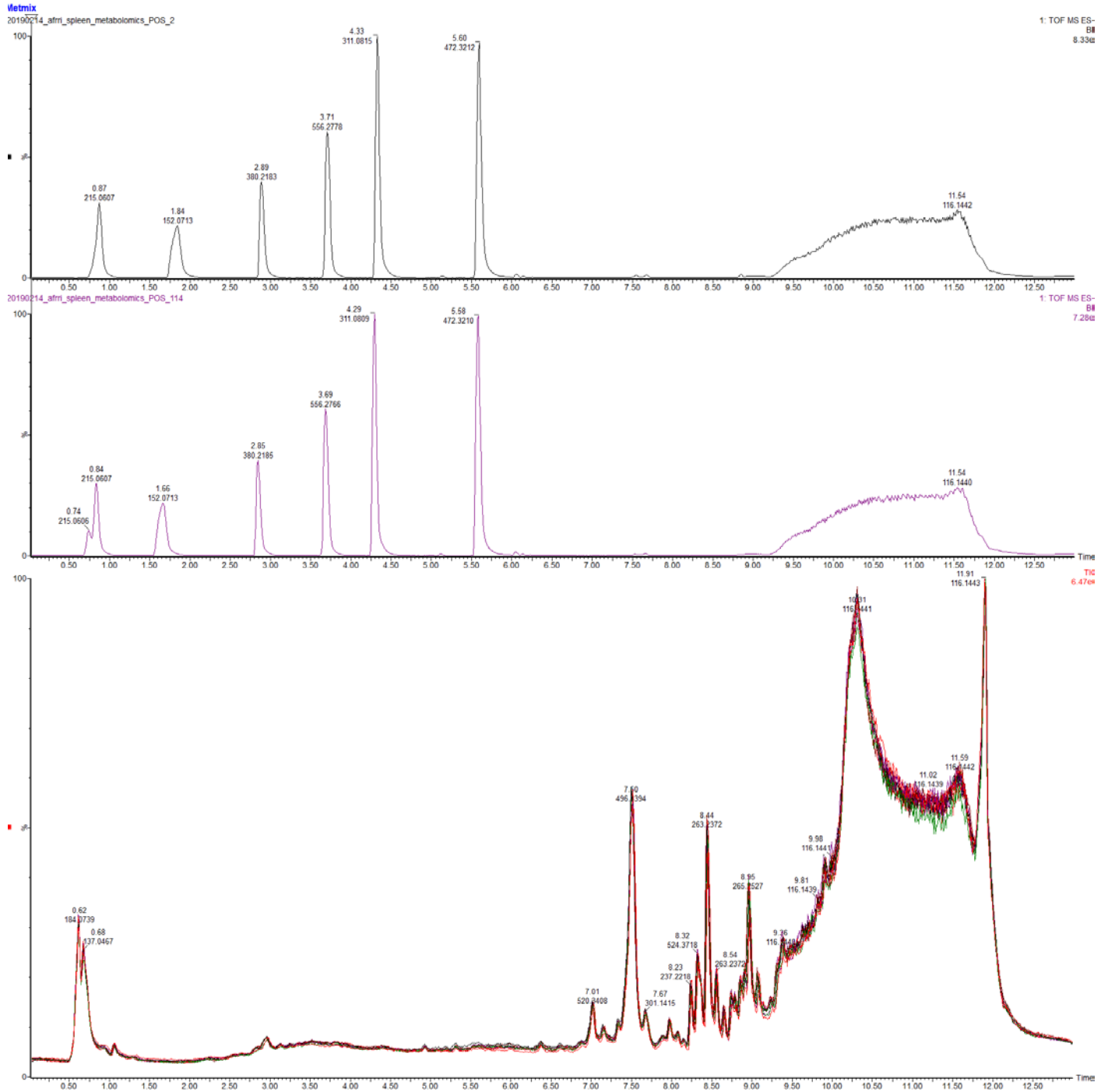
Supplementary Figure 1

A

Name	POS	Initial INPUT	PPM error
Acetaminophen	152.0712	152.0713	0.65
Sulfaguanidine	215.0603	215.0607	1.85
Sulfadimethoxine	311.0814	311.0815	0.32
Val-Tyr-Val	380.2185	380.2183	-0.52
Terfenadine	472.3216	472.3212	-0.84
Leu-Enkephalin	556.2771	556.2778	1.25

Name	POS	Final INPUT	PPM error
Acetaminophen	152.0712	152.0713	0.65
Sulfaguanidine	215.0603	215.0608	2.32
Sulfadimethoxine	311.0814	311.0809	-1.6
Val-Tyr-Val	380.2185	380.2185	0
Terfenadine	472.3216	472.321	-1.27
Leu-Enkephalin	556.2771	556.2766	-0.89

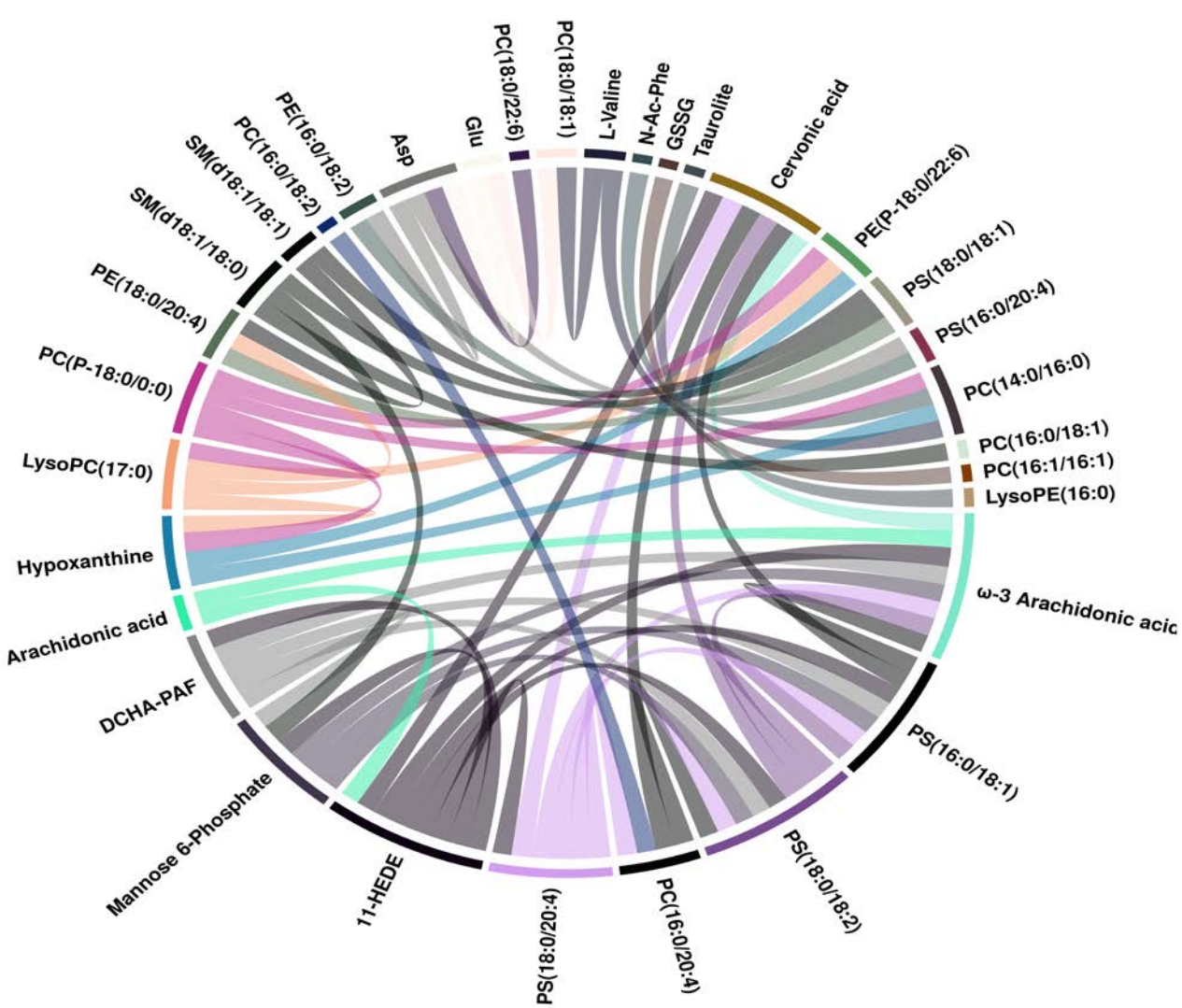
B



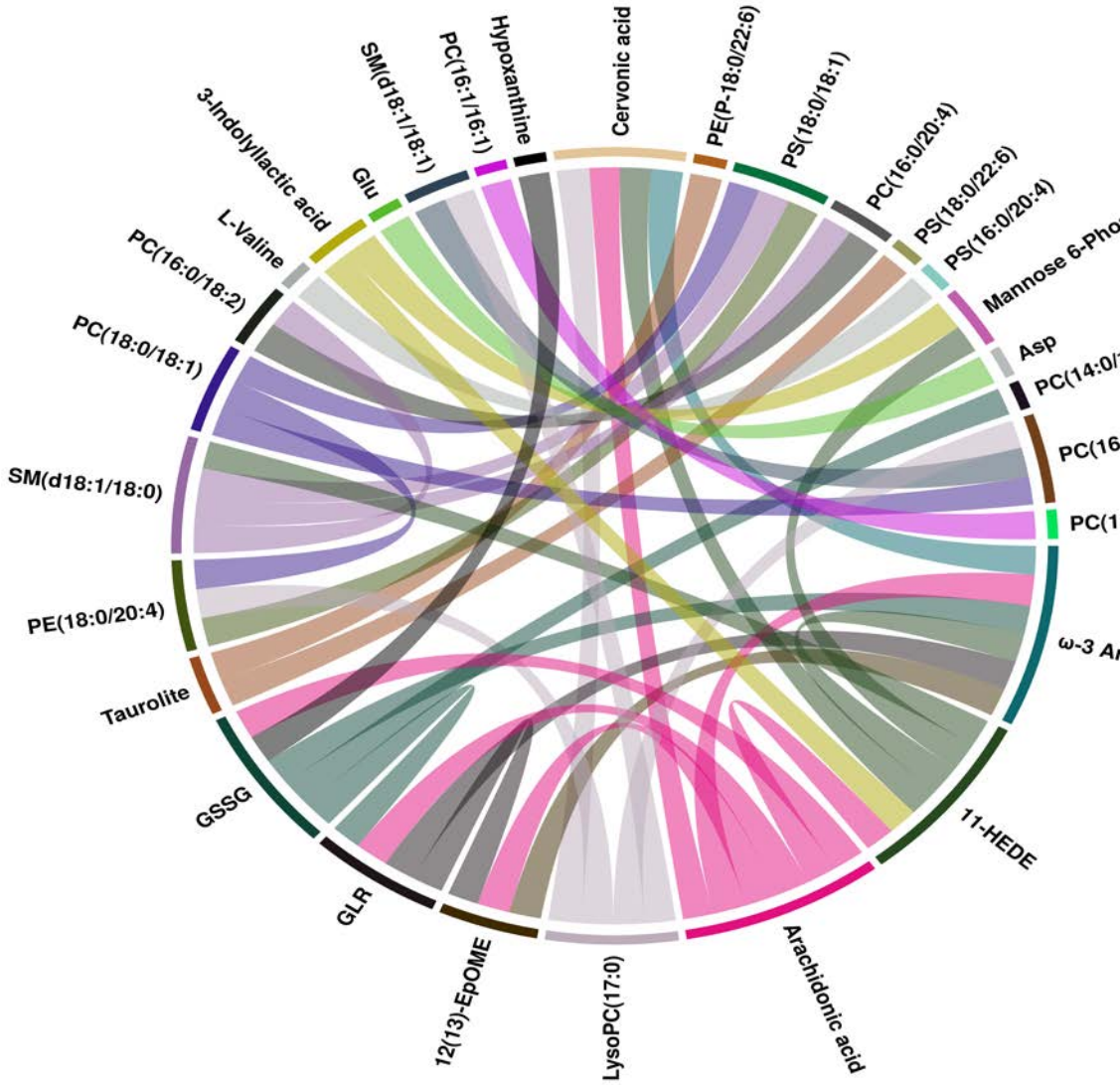
Supplementary Figure 1: A) Mass accuracy checks were performed at the beginning and end of the batch using a mix of 6 standard compounds. The ppm mass accuracy checks for these 6 compounds were all within 5 ppm for both positive and negative ionization modes. **B)** Chromatograms of the mass accuracy checks at the beginning (top) and the end (bottom) of a batch. **C)** Overlay of all pooled QC samples throughout a batch show minimum shifts in retention times and intensities.

Supplementary Figure 2

Vehicle

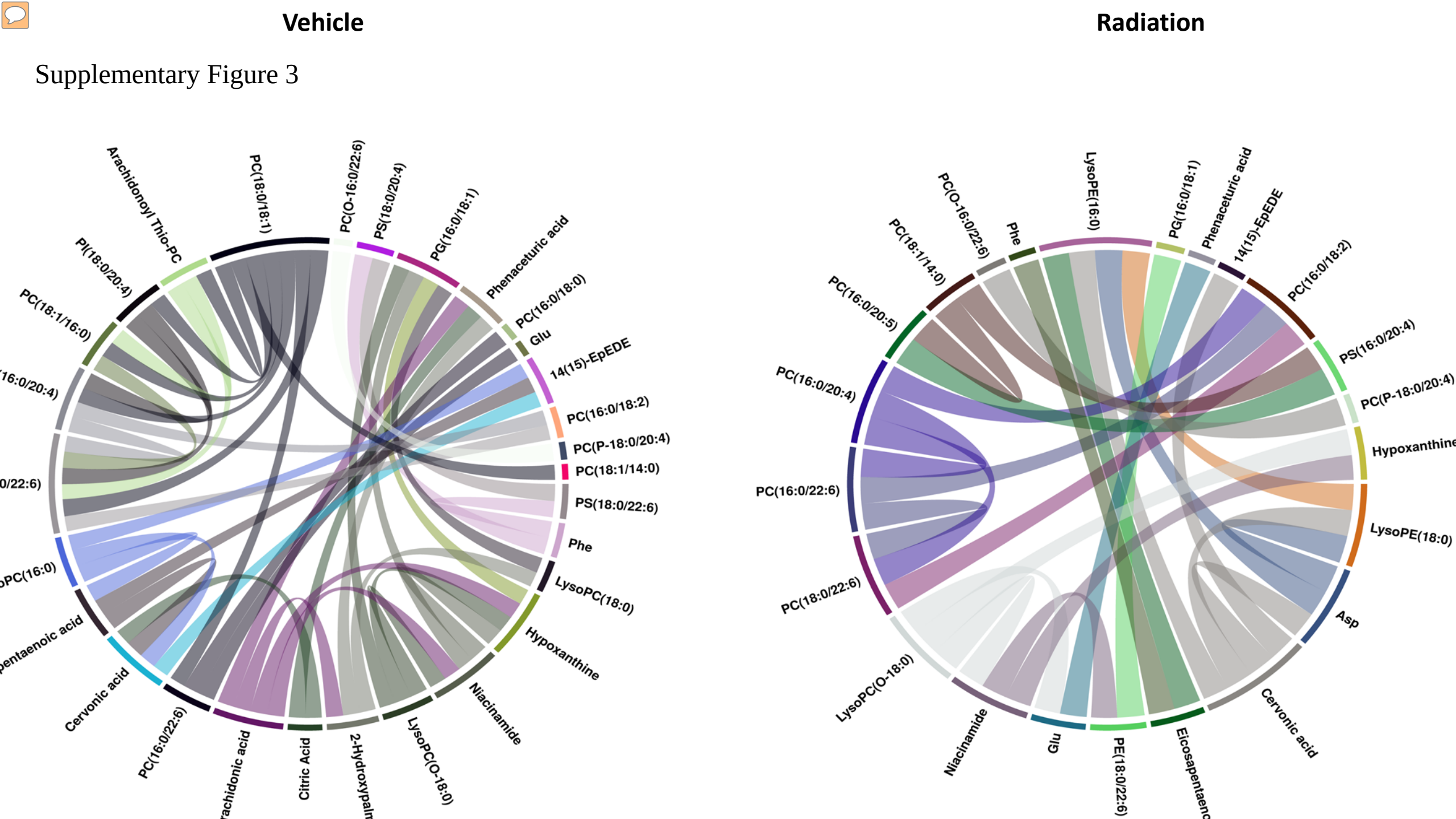


Radiation



Supplementary Figure 2: Circos plot for identified metabolites and their correlations before (Panel A) and after (Panel B) radiation expose at SD4 in spleen tissue. This figure illustrates the dysregulating impact of ionizing radiation on the metabolic profiles. Each band in the plot represents a statistical measure of the strength of a monotonic relationship between paired metabolites. Spearman correlation coefficient was set to a minimum of 0.5 and the p value < 0.01.

Supplementary Figure 3



Supplementary Figure 3: Circos plot for identified metabolites and their correlations before (Panel A) and after (Panel B) radiation expose at SD4 for kidney tissue. This figure illustrates the dysregulating impact of ionizing radiation on the metabolic profiles. Each band in the plot represents a statistical measure of the strength of a monotonic relationship between paired metabolites. Spearman correlation coefficient was set to a minimum of 0.5 and the p value < 0.01.

Supplementary Table 1. Table of Tandem MS Validated Metabolites

Name	Ionization Mode	Matrix	precursor mz	rt	Synonyms	Adduct	Level	CID	Class	
N-(1-Oxo-5Z,8Z,11Z,14Z-eicosatetraenyl)-L-alanine	Positive	Heart	375.2612	7.63	N-Arachidonoyl-L-alanine	[M+H]+	1	375.26, 287.26, 269.22, 245.22, 213.16, 203.17, 185.13, 171.11, 147.11, 131.1, 119.08, 105.06, 95.08, 81.06	N-Acyl Amino Acids	
1-Glyceryl oleate	Positive	Heart	357.2772	8.9	Monoolein	[M+H]+	1	357.29, 339.29, 265.25, 177.16, 149.13, 135.11, 121.1, 109.1, 95.08, 81.07, 69.07	Monoglycerides	
DL-2-Aminovaleric acid	Positive	Heart	118.0874	0.43	DL-Norvaline	[M+H]+	1	118.08, 72.08	Amino Acids	
L-Glutamine	Positive	Heart	147.0776	0.44	Gln	[M+H]+	1	147.06, 130.06, 84.04	Amino Acids	
cis-5,8,11,14-Eicosatetraenoic acid	Positive	Heart	305.2484	8.02	Arachidonic acid	[M+H]+	1	305.24, 287.23, 269.22, 245.22, 221.15, 177.16, 147.11, 121.1, 95.08	Fatty Acids And Derivatives	
(3R)-3-Hydroxy-4-(trimethylammonio)butanoate	Positive	Heart	162.1136	0.41	L-Carnitine	[M+H]+	1	162.11, 103.03, 85.08, 60.08	Amino Acids	
(alpha-Methylguanido)acetic acid	Positive	Heart	132.0778	0.42	Creatine	[M+H]+	1	132.07, 114.06, 90.05	Amino Acidds	
L-Glutamic acid	Positive	Heart	148.0049	0.43	Glu	[M+H]+	1	148.00, 130.05, 102.05, 84.04	Amino Acids	
1-Stearoyl-2-hydroxy-sn-alvcero-3-ohosohocholine	Positive	Heart	524.3713	7.46	LvsoPC(18:0)	[M+H]+	1	524.37. 306.36. 341.3. 184.07. 104.1	Phosphatidylchlines	
Docosahexaenoic acid methyl ester	Positive	Heart	342.203	9.11	Methyl DHA	[M+2H]+	1	345.2787,344.2668,343.2641,311.2384,301.2101,161.1316,145.1016,133.1013,131.0855,121.1017,119.0858,107.0856,105.07,95.0859,93.07	Fatty Acids And Derivatives	
Adenosine 5'-monophosohate	Positive	Heart	348.0715	0.45	5'-Adenvlic acid	[M+H]+	2	348.07. 137.04. 136.06119.03. 97.02	Nucleoside Monophosohate	
1-Palmitoyl-sn-glycero-3-phosphocholine	Positive	Heart	991.6712	6.71	LysoPC(16:0)	[2M+H]+	2	991.67, 590.32, 496.34, 184.07, 104.08	Lysophosphatidylcholine	
1-Stearoyl-2-hydroxy-sn-alvcero-3-ohosohoethanolamine	Positive	Heart	482.3248	7.43	LvsoPE(18:0)	[M+H]+	2	482.32. 464.31. 421.27. 341.3. 310.31.	Lysophosohatidylethanolamine	
N-(Eicosanoyl)sphingosine	Positive	Heart	575.5029	10.8	Cer(d18:1/20:0)	[M+H-H2O]+	2	575.5, 282.22, 264.27, 262.25, 252.26,	Ceramides	
N-(11R)-2-Hydroxy-1-methylethyl-9Z-octadecenamide	Positive	Heart	323.2528	8.15	Methvl oleovlethanolamide	[M+H-H2O]+	2	323.25. 263.23. 245.22. 191.17. 177.2. 163.2. 149.132. 135.17. 121.05. 109.1. 97.1.	N-Acvl Amino Acids	
cis-4,7,10,13,16,19-Docosahexaenoic acid	Positive	Heart	329.2477	7.48	Cervonic acid	[N+H]+	2	329.24, 293.22, 269.22, 247.16, 215.17, 201.16, 175.14, 159.11, 145.1, 133.1, 119.08, 107.08, 96.08, 81.06	Fatty Acids And Derivatives	
Docosapentaenoic acidmethyl ester	Positive	Heart	344.2587	8.67	Methyl DPA	[M+2H]+	2	344.25, 311.23, 293.232, 287.23, 283.21, 273.19, 269.22, 255.17, 261.18, 241.16, 215.16, 201.16, 175.14, 161.13, 133.1, 93.07, 67.05	Fatty Acids And Derivatives	
8Z,14Z-Eicosadienoic acid	Positive	Heart	291.2665	8.27	Eicosadienoic acid	[M+H-H2O]+	2	291.26, 147.11, 123.11, 109.1, 95.08, 81.07, 67.05	Fatty Acids And Derivatives	
Ricinoleic acid methyl ester	Positive	Heart	313.2739	8.01	Methyl ricinoleate	[M+H]+	2	313.27, 295.26, 263.23, 245.22	Fatty Acids And Derivatives	
cis-8,11,14-Eicosatrienoic acid	Positive	Heart	307.2588	8.32	γ-Homolinolenic acid	[M+H]+	2	307.25, 289.25, 209.14, 173.13, 109.1, 96.08, 81.07	Fatty Acids And Derivatives	
2-Arachidonoylglycerol	Positive	Heart	379.2825	8.14	2-AG	[M+H]+	2	379.28, 305.24, 287.23, 269.22, 245.22, 203.17	Monoglycerides	
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Positive	Heart	454.3896	6.9	LysoPE(16:0)	[M+H]+	2	454.38, 313.27, 155.02, 85.02	Lysophosphatidylethanolamine	
cis-7,10,13,16-Docosatetraenoic acid	Positive	Heart	333.2791	8.5	Adrenic Acid (22:4, n-6)	[M+H]+	2	33.27, 249.18, 205.19, 135.11, 121.1	Fatty Acids And Derivatives	
13-Docosenamide, (Z)-	Positive	Heart	338.1829	8.61	Erucamide	[M+H]+	2	338.18, 303.3, 163.14, 135.1, 121.1, 109.1, 95.08, 81.07	Fatty Acids And Derivatives	
5-Heptenoic acid, 7-[(1R,4S,5S,6R)-6-[(1E,,3S,5Z)-3-hydroxy-1,5-octadien-1-yl]-2-oxabicyclo[2.2.1]hept-5-yl]-, (5Z)-	Positive	Heart	331.2637	8.11	DELTA.17-U-46619	[M+H-H2O]+	2	331.26, 239.14, 135.11, 121.1, 109.1, 95.08, 81.08	Prostaglandins And Derivatives	
1-Hexadecanoyl-2-octadecadienoyl-sn-glycero-3-phosphocholine	Positive	Heart	758.5699	9.87	PC(16:0/18:2)	[M+H]+	2	758.56, 184.07, 86.09	Phosphatidylcholine	
1,2-Dipalmitoleoyl-sn-glycero-3-phosphocholine	Positive	Heart	730.5382	9.74	PC(16:1/16:1)	[M+H]+	2	730.53, 184.07, 86.09	Phosphatidylcholine	
1-Palmitoyl-2-oleoyl-phosphatidylglycerol	Positive	Heart	771.5146	11.04	PG(16:0/18:1)	[M+Na]+	2	771.52, 577.2, 195.08, 67.05	Phosphatidylglycerol	
1,2-Dilinoleoyl-sn-glycero-3-phospho-(1'-rac-glycerol)	Positive	Heart	793.5039	11.59	PG(18:2)	[M+Na]+	2	793.5, 195.08	Diglycerides	
1,2-Dioleoyl-sn-glycero-3-phospho-rac-1-glycerol	Positive	Heart	797.5311	11.06	PG(18:1/18:1)	[M+Na]+	2	797.53, 195.00	Diglycerides	
N-[1-Oxo-5Z,8Z,11Z,14Z-eicosatetraenyl]-L-serine	Positive	Heart	287.2357	8.02	N-Arachidonoyl-L-serine	[M+H-C3H7O3N]+	2	287.23, 269.22, 203.17, 171.11, 148.97, 131.04, 119.08	N-Acyl Amino Acids	
1-Octadecanoyl-2-octadecenoyl-sn-glycero-3-phosphocholine	Positive	Heart	810.5073	9.69	PC(18:0/18:1)	[M+Na]+	2	810.5, 184.07	Phosphatidylchlines	
Arachidonoylthiophosphorylcholine	Positive	Heart	784.5823	9.86	Arachidonoyl Thio-PC	[M+H]+	2	784.56, 184.07	Thiophospholipids	
2-Docosahexaenoyl-1-stearoyl-sn-alvcero-3-ohosohoethanolamine	Positive	Heart	792.5703	9.89	PE(18:0/22:6)	[M+H]+	2	792.57. 651.53	Phosphatidylethanolamine	
6H-Purin-6-one, 1,7-dihydro-	Positive	Heart	137.047	0.47	Hypoxanthine	[M+H]+	2	137.04., 119.03, 110.03, 82.03	Purine Derivative	Might indicate DNA damage
7α,12α-Dihvdroxvcholest-4-en-3-one	Positive	Heart	400.2676	7.69	7α,12α-Dihvdroxvcholest-4-en-3-one	[M+H-H2O]+	3	400.28. 269.22. 227.17. 185.12. 159.11. 131.07. 93.06	7Alpha-Hydroxv Steroid	
9(10)-Epoxy-12Z-octadecenoic acid	Positive	Heart	279.2321	7.69	9(10)-EpOME	[M+H-H2O]+	3	279.23, 173.13, 149.13, 135.16, 123.18, 104.1	Fatty Acids And Derivatives	
15(R).19(R)-Hydroxvprostaglandin E1	Positive	Heart	353.2668	8.12	15.19-Hhvdroxv PGE1	[M+H-H2O]+	3	353.26. 263.23. 245.22. 121.1. 95.08. 81.08	Prostaglandins And Derivatives	
1-Palmitoyl-2-stearoyl-sn-glycero-3-phosphocholine	Positive	Heart	762.5126	9.67	PC(16:0/18:0)	[M+H]+	3	762.51, 184.07	Phosphatidylchlines	
9Z.12Z-Octadecadienoic acid. 2-vlcervl ester®	Positive	Heart	355.2837	7.63	2-Linoleovlglycerol	[M+H]+	1	355.28. 337.27. 263.23. 245.22. 189.16. 175.14. 149.13. 135.11. 121.1. 95.08. 81.06	Monoglycerides	
1-Propanaminium, 2-(acetyloxy)-3-carboxy-N,N,N-trimethyl-, inner salt	Positive	Heart	204.1241	0.44	Acetylcarnitine	[M+H]+	1	204.13, 145.04, 85.02	Miscellaneous	
Palmitoyleicosapentaenoyl phosphatidylcholine	Positive	Heart	780.5537	9.7	PC(16:0/20:5)	[M+H]+	2	780.55, 184.07	Phosphatidylcholine	
2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine	Positive	Heart	760.5854	9.96	PC(16:0/18:1)	[M+H]+	2	760.58, 184.07	Phosphatidylcholine	
1-Docosahexaenoyl-2-stearoyl-sn-glycero-3-phosphocholine	Positive	Heart	834.6007	9.89	PC(22:6/18:0)	[M+H]+	2	834.6, 184.07	Phosphatidylcholine	
1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine	Positive	Heart	806.5694	9.78	PC(16:0/22:6)	[M+H]+	2	806.56, 184.07	Phosphatidylcholine	
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Negative	Kidney	480.309	8.31	LysoPE(18:0)	[M-H]-	2	480.3, 283.26, 196.03, 140.01, 78.95	Phosphatidylethanolamine And Derivatives	
L-Glutamic acid	Negative	Kidney	146.045	0.62	Glu	[M-H]-	1	146.04, 128.03, 102.05, 85.02	Amino Acids And Derivatives	
2-Hydroxypalmitic acid	Negative	Kidney	271.2269	8.59	2-Hydroxypalmitic acid	[M-H]-	1	271.2273, 225.2225	Fatty Acids And Derivatives	
1,2,3-Propanetricarboxylic acid, 2-hydroxy-	Negative	Kidney	191.0187	0.7	Citric Acid	[M-H]-	1	191.01, 129.01, 111.09, 87.01, 85.02	Miscellaneous	
1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phosphocholine	Negative	Kidney	826.5608	10.2	PC(16:0/20:4)	[M+HCO2]-	1	826.5570, 766.5362, 480.3084, 303.2321, 255.2321	Phosphatidylcholine And Derivatives	
1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine	Negative	Kidney	802.5607	10.25	PC(16:0/18:2)	[M-H]-	2	802.56, 742.53, 480.3, 391.22, 279.23, 255.23	Phosphatidylcholine And Derivatives	
Carbocyclic thromboxane A2	Negative	Kidney	329.2477	9.03	Carbocyclic thromboxane A2	[M-H-H2O]-	1	329.2470, 285.2580, 231.2046	Miscellaneous	
cis-4,7,10,13,16,19-Docosahexaenoic acid	Negative	Kidney	327.232	8.65	Cervonic acid	[M-H]-	2	327.23, 309.2, 283.24, 249.18, 229.19, 191.18, 177.16	Fatty Acids And Derivatives	
1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine	Negative	Kidney	850.5611	10.15	PC(16:0/22:6)	[M-H]-	2	850.56, 790.54, 480.3, 327.23, 283.24	Phosphatidylcholine And Derivatives	
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phospho-(1'-myo-inositol)	Negative	Kidney	886.6084	10.37	PI(18:0/20:4)	[M-2H]-	2	886.6, 419.25, 283.26	Phosphatidylinositol And Derivatives	
1-Oleoyl-2-palmitoyl-sn-glycero-3-phosphocholine	Negative	Kidney	804.5756	10.35	PC(18:1/16:0)	[M+H]+	2	804.57, 744.55, 281.24, 255.23	Phosphatidylcholine And Derivatives	
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Negative	Kidney	452.2776	7.48	LysoPE(16:0)	[M-H]-	2	452.27, 255.23, 196.04	Phosphatidylethanolamine And Derivatives	
8,11-Tridecadienoic acid, 13-(3-pentyl-2-oxiranyl)-, (8Z,11Z)-	Negative	Kidney	303.2321	8.79	14(15)-EpEDE	[M-H-H2O]-	1	303.2325, 285.2220, 259.2429, 231.2116, 191.1077, 177.0919, 163.0764	Fatty Acids And Derivatives	
1-Stearoyl-2-docosahexaenoyl-sn-alvcero-3-ohosohocholine	Negative	Kidney	878.5919	10.26	PC(18:0/22:6)	[M+HCO2]-	1	878.5917. 818.5676. 508.3403. 327.2319. 283.2632	Phosphatidylcholine And Derivatives	
1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Negative	Kidney	781.4888	11.91	PS(16:0/20:4)	[M-2H]-	2	781.48, 605.48, 439.22, 391.22, 303.23, 255.23	Phosphatidylserine And Derivatives	
1-Stearoyl-2-hydroxy-sn-alvcero-3-ohosohocholine	Negative	Kidney	568.2675	7.42	LvsoPC(18:0)	[M+Formic-H]-	2	568.26. 508.33. 419.25. 283.26. 224.06. 152.99	Phosphatidylcholine And Derivatives	
2-Docosahexaenoyl-1-stearoyl-sn-glycero-3-phosphoserine	Negative	Kidney	834.5288	11.91	PS(18:0/22:6)	[M-H]-	2	834.52, 747.49, 403.22, 419.25, 283.26, 152.99	Phosphatidylserine And Derivatives	
Glycine. N-(2-phenylacetyl)-	Negative	Kidney	192.0654	3.15	Phenaceturic acid	[M-H]-	1	192.06. 74.02	Amino Acids And Derivatives	
1-Palmitoyl-2-oleoyl-phosphatidylglycerol	Negative	Kidney	747.5197	10.26	PG(16:0/18:1)	[M-H]-	2	747.51, 281.24, 152.99	Phosphatidylglycerol And Derivatives	
1-Palmitoyl-2-stearoyl-sn-elvcero-3-ohosohocholine	Negative	Kidney	806.5851	10.39	PC(16:0/18:0)	[M+HCO2]-	1	806.5887. 746.5676. 480.3088. 283.2633. 255.2320	Phosphatidylcholine And Derivatives	
L-Aspartic acid	Negative	Kidney	132.0292	0.62	Asp	[M-H]-	2	132.02, 115, 88.04, 71.01	Amino Acids And Derivatives	
2-Docosahexaenoyl-1-stearoyl-sn-glycero-3-phosphoethanolamine	Negative	Kidney	790.5385	10.3	PE(18:0/22:6)	[M-H]-	2	790.53, 480.3, 327.23, 283.26	Phosphatidylethanolamine And Derivatives	
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Negative	Kidney	810.5296	11.92	PS(18:0/20:4)	[M-H]-	2	810.52, 723.49, 419.25, 283.26, 152.99	Phosphatidylserine And Derivatives	
1-Octadecanoyl-sn-glycero-3-phosphoserine	Negative	Kidney	524.2986	12.01	PS(18:0/0:0)	[M-H]-	2	524.29, 437.26, 152.99	Phosphatidylserine And Derivatives	
1-(1Z-octadecenyl)-2-docosahexaenoyl-sn-glycero-3-phosphoethanolamine	Negative	Kidney	464.3138	8.52	PE(P-18:0/22:6)	[M-H]-	2	464.3165, 267.2704, 196.0388, 140.0125, 78.9594	Phosphoethanolamine And Derivatives	
cis-5,8,11,14,17-Eicosapentaenoic acid	Positive	Kidney	303.2307	8.38	Eicosapentaenoic acid	[M+H]+	2	303.23, 163.14, 147.17, 121.1, 96.07	Fatty Acids And Derivatives	
2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine	Positive	Kidney	782.5704	10.25	PC(18:0/18:1)	[M+H]+	2	782.57, 184.07, 86.09	Phosphatidylcholine And Derivatives	
DL-Phenylalanine	Positive	Kidney	166.0862	1.11	Phe	[M+H]+	1	166.08, 120.08, 103.05	Amino Acids And Derivatives	
6H-Purin-6-one, 1,7-dihydro-	Positive	Kidney	137.0462	0.72	Hypoxanthine	[M+H]+	1	137.27, 137.04, 119.03, 110.03, 82.01	Miscellaneous	
Niacinamide	Positive	Kidney	123.0415	0.69	Niacinamide	[M+H]+	1	123.04, 96.04, 80.04	Miscellaneous	
1-Palmitoyl-sn-glycero-3-phosphocholine	Positive	Kidney	518.3202	7.49	LysoPC(16:0)	[M+H]+	2	518.32, 459.24, 313.27, 146.98	Phosphatidylcholine And Derivatives	
cis-5,8,11,14-Eicosatetraenoic acid	Positive	Kidney	305.2473	8.78	Arachidonic acid	[M+H]+	1	305.24, 287.23, 269.22, 245.22, 147.11, 121.1, 93.07	Fatty Acids And Derivatives	
1-O-Octadecyl-sn-glycervl-3-phosphorylcholine	Positive	Kidney	510.3542	7.88	LysoPC(O-18:0)	[M+H]+	2	510.35, 184.07, 125, 104.1, 86.09	Phosphatidylcholine And Derivatives	
Palmitoyleicosapentaenoyl phosphatidylcholine	Positive	Kidney	780.5565	10.15	PC(16:0/20:5)	[M+H]+	2	780.56, 184.07	Phosphatidylcholine And Derivatives	
Arachidonoylthiophosphorylcholine	Positive	Kidney	784.5822	10.28	Arachidonoyl Thio-PC	[M+H]+	2	784.58, 184.07	Phosphatidylcholine And Derivatives	
1,2-Dipalmitoleoyl-sn-glycero-3-phosphocholine	Positive	Kidney	730.545	10.19	PC(16:1/16:1)	[M+H]+	2	730.54, 184.07	Phosphatidylcholine And Derivatives	
1-(1Z-Octadecenyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine	Positive	Kidney	794.5986	10.27	PC(P-18:0/20:4)	[M+H]+	2	794.58, 184.07	Phosphatidylcholine And Derivatives	
1-O-Hexadecyl-2-O-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycervl-3-phosphorylcholine	Positive	Kidney	792.59	10.26	PC(O-16:0/22:6)	[M+H]+	2	792.59, 184.07	Phosphatidylcholine And Derivatives	
1-Oleovl-2-mvristovl-sn-alvcero-3-ohosohocholine	Positive	Kidney	732.5564	10.31	PC(18:1/14:0)	[M+H]+	2	732.55. 184.07	Phosphatidylcholine And Derivatives	
N-(Octadecanoyl)sphing-4-enine-1-phosphocholine	Positive	Kidney	731.5898	10.4	Sphingomyelin	[M+H]+	2	731.58, 184.07	Sphingomyelin	
12(13)-Epoxy-9Z-octadecenoic acid	Neeative	Soleen	295.227	7.22	12(13)-EpOME	[M-H]-	2	195.22. 277.21. 195.13. 183.01. 171.1	Fatty Acis And Derivative	
L-Aspartic acid	Negative	Spleen	132.0293	0.62	Asp	[M-H]-	2	132.03, 115, 88.04, 71.01	Amino Acid And Derivatives	
cis-4.7.10.13.16.19-Docosahexaenoic acid	Neeative	Soleen	327.2322	8.65	Cervonic acid	[M-H]-	2	327.23. 249.17. 229.19. 177.16	Fatty Acis And Derivative	
L-Glutamic acid	Negative	Soleen	146.0449	0.62	Glu	[M-H]-	2	146.04, 128.04, 102.06	Amino Acid And Derivatives	
D-Mannose 6-ohosohate	Negative	Soleen	259.0216	0.66	Mannose 6-Phosohate	[M-H]-	2	259.02. 168.99. 96.96. 78.95	Miscellaneous	
1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine	Negative	Spleen	802.5608	10.24	PC(16:0/18:2)	[M+Formic]-	2	802.56, 742.53, 480.3, 391.22, 279.23, 255.23	Phosphatidylcholine And Derivatives	
1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phosphocholine	Negative	Spleen	826.5609	10.2	PC(16:0/20:4)	[M-H]-	3	826.56, 766.53	Phosphatidylcholine And Derivative	
2-Linoleoyl-1-palmitoyl-sn-glycero-3-phosphoethanolamine	Negative	Spleen	714.5079	10.31	PE(16:0/18:2)	[M-H]-	2	714.5, 452.27, 279.23, 255.23	Phosphatidylethanolamine And Derivatives	
2-Arachidonoyl-1-palmitoyl-sn-glycero-3-phosphoethanolamine	Negative	Spleen	738.5085	10.27	PE(16:0/20:4)	[M-H]-	2	738.5, 500.27, 452.27, 303.23, 255.23	Phosphatidylethanolamine And Derivatives	
2-Arachidonoyl-1-stearoyl-sn-glycero-3-phosphoethanolamine	Negative	Spleen	520.2662	7.46	PE(18:0/20:4)	[M-H]-	2	766.53, 480.3, 303.23	Phosphatidylethanolamine And Derivatives	
1-(1Z-Octadecenyl)-2-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphoethanolamine	Negative	Spleen	464.312	7.87	PE(P-18:0/22:6)	[M-H]-	2	464.31, 267.27, 196.03, 140.01, 78.95	Phosphatidylethanolamine And Derivatives	
2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphoserine	Negative	Spleen	760.5127	11.91	PS(16:0/18:1)	[M-H]-	2	760.5, 673.47, 391.22, 152.99	Phosphatidylserine And Derivative	
1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Negative	Spleen	782.4981	11.91	PS(16:0/20:4)	[M-H]-	2	782.49, 695.46, 391.22, 255.23	Phosphatidylserine And Derivative	
2-Oleoyl-1-stearoyl-sn-glycero-3-phosphoserine	Negative	Spleen	788.5428	11.9	PS(18:0/18:1)	[M-H]-	2	788.54, 701.51, 419.25, 283.26	Phosphatidylserine And Derivative	
1-Stearoyl-2-linoleoyl-sn-glycero-3-phospho-L-serine	Negative	Spleen	786.5289	11.91	PS(18:0/18:2)	[M-H]-	2	786.52, 699.49, 419.25, 283.26, 152.99, 78.95	Phosphatidylserine And Derivative	
1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine	Negative	Spleen	810.5295	11.91	PS(18:0/20:4)	[M-H]-	2	810.52, 723.49, 419.25, 283.26, 152.99, 78.95	Phosphatidylserine And Derivative	
2-Docosahexaenoyl-1-stearoyl-sn-glycero-3-phosphoserine	Negative	Spleen	834.6138	10.43	PS(18:0/22:6)	[M-H]-	2	834.61, 147.49, 419.25, 283.26, 152.99, 78.95	Phosphatidylserine And Derivative	
8Z,11Z,14Z,17Z-Eicosatetraenoic acid	Negative	Spleen	303.2321	8.8	ω-3 Arachidonic acid	[M-H]-	2	303.23, 285.22, 259.24, 205.19	Fatty Acis And Derivative	
11-Hydroxy-12E,14Z-eicosadienoic acid	Positive	Spleen	307.2567	9.03	11-HEDE	[M+H]+	1	307.26, 289.24, 209.17, 149.12, 137.13, 123.11, 109.1, 95.08, 81.07, 67.05	Fatty Acis And Derivative	
DL-Indole-3-lactic acid	Positive	Spleen	206.0677	0.64	3-Indolyllactic acid	[M+H]+	2	206.06, 188.07, 146.06, 118.06	Miscellaneous	
cis-5,8,11,14-Eicosatetraenoic acid	Positive	Spleen	305.2477	8.8	Arachidonic acid	[M+H]+	1	305.24, 287.23, 269.22, 259.2, 245.22, 221.15, 147.11, 121.1,	Fatty Acis And Derivative	
Arginine	Positive	Spleen	175.0747	0.63	Arg	[M+H]+	3	175.11, 116.07, 70.06	Amino Acids And Derivatives	
Docosahexaenoyl PAF C-16	Positive	Spleen	792.5738	10.28	DCHA-PAF	[M+H]+	2	792.57, 184.07	Phosphatidylcholine And Derivative	
Glv-Leu-Are	Positive	Spleen	173.0806	0.85	GLR	[M+2H]2+	2	173.08. 158.08. 116.06. 112.04. 86.1. 70.06. 60.05	Short Peptides	
Glutathione, oxidized	Positive	Spleen	613.1586	0.69	GSSG	[M+H]+	1	613.15, 638.13, 484.11, 409.08, 355.07, 288.06, 231.04, 177.03, 130.04	Miscellaneous	
6H-Purin-6-one. 1.7-dihvdro-	Positive	Spleen	137.0466	0.7	Hvpoxanthine	[M+H]+	2	137.04. 119.03. 110.03. 82.04	Miscellaneous	
(S)-2-Amino-3-methylbutanoic acid	Positive	Spleen	118.0867	0.67	L-Valine	[M+H]+	2	118.08, 72.08	Amino Acids And Derivatives	

1-Heptadecanoyl-sn-glycero-3-phosphocholine	Positive	Spleen	510.355	7.9	LysoPC(17:0)	[M+H]+	2	510.35, 184.07, 124.99, 104.1, 88.09	Phosphatidylcholine And Derivative
1-Behenoyl-2-hydroxy-sn-glycero-3-phosphocholine	Positive	Spleen	580.3577	9.64	LysoPC(22:0)	[M+H]+	2	580.35. 184.07. 104.07	Phosphatidylcholine And Derivative
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	Positive	Spleen	476.2791	7.46	LysoPE(16:0)	[M+H]+	2	476.27, 433.23	Phosphatidylethanolamine And Derivatives
N-Acetyl-L-phenylalanine	Positive	Spleen	165.0544	0.71	N-Ac-Phe	[M+-Acl+	2	165.08. 149.05. 120.08. 103.05. 93.06. 77.03	Amino Acids And Derivatives
1-Myristoyl-2-palmitoyl-sn-glycero-3-phosphocholine	Positive	Spleen	706.5434	10.3	PC(14:0/16:0)	[M+H]+	2	706.54, 184.07, 86.09	Phosphatidylcholine And Derivative
2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine	Positive	Spleen	760.5845	10.36	PC(16:0/18:1)	[M+H]+	2	760.58, 184.07	Phosphatidylcholine And Derivative
1,2-Dipalmitoleoyl-sn-glycero-3-phosphocholine	Positive	Spleen	730.544	10.2	PC(16:1/16:1)	[M+H]+	2	730.54, 184.07	Phosphatidylcholine
1-Octadecanoyl-2-octadecenoyl-sn-glycero-3-phosphocholine	Positive	Spleen	810.6004	10.33	PC(18:0/18:1)[]	[M+H]+	2	810.58, 751.52, 184.07, 146.98	Phosphatidylcholine And Derivative
1-Docosahexaenoyl-2-stearoyl-sn-glycero-3-phosphocholine	Positive	Spleen	834.5996	10.25	PC(18:0/22:6)	[M+H]+	2	834.599, 184.07	Phosphatidylcholine And Derivative
1-Oleoyl-2-myristoyl-sn-glycero-3-phosphocholine	Positive	Spleen	732.5571	10.3	PC(18:1/14:0)	[M+H]+	2	732.55, 184.07	Phosphatidylcholine And Derivative
1-(1Z-Octadecenyl)-sn-glycero-3-phosphocholine	Positive	Spleen	508.372	7.89	PC(P-18:0/0:0)	[M+H]+	2	508.37, 184.07, 125, 104.1, 86.09	Phosphatidylcholine And Derivative
N-Oleoyl-D-erythro-sphingosylphosphorylcholine	Positive	Spleen	729.5727	10.38	SM(d18:1/18:1)	[M+H]+	2	729.59, 184.07	Sphingomyelin
N-(Octadecanoyl)sphing-4-enine-1-phosphocholine	Positive	Spleen	731.5945	10.43	SM(d18:1/18:0)	[M+H]+	2	731.6, 184.07	Sphingomyelins[]
Tauroursodeoxycholic acid	Positive	Spleen	482.324	8.33	Taurolite	[M+H-H2O]+	2	482.32, 464.31	Bile Acid Conjugates

Supplementary Table 2. Radiation effects Metabolites

Radiation effect at SD 4 and SD 9 for validated metabolites across all tissues

			SD 4				SD 9			
			Rad/Vehicle				Rad/Vehicle			
Name	**Matrix**	**Ionization Mode**	***p-value***	***FDR*** [a]	***Fold Change***	***log2(FC)***	***p-value***	***FDR***	***Fold Change***	***log2(FC)***
PC(16:0/18:2)	Heart	Positive	2.97E-04	5.20E-03	0.78077	-0.35704	NS	NS	1.0147	0.020996
PC(16:0/20:5)	Heart	Positive	1.17E-02	NS	0.86089	-0.2161	NS	NS	0.84106	-0.24972
Arachidonoyl Thio-PC	Heart	Positive	NS	NS	0.92349	-0.11484	4.12E-03	NS	1.2167	0.28302
PC(16:1/16:1)	Heart	Positive	1.34E-03	1.46E-02	0.75197	-0.41125	NS	NS	0.89575	-0.15884
PE(18:0/22:6)	Heart	Positive	5.45E-04	7.79E-03	1.4382	0.52426	NS	NS	1.0307	0.043632
PC(16:0/18:0)	Heart	Positive	4.71E-03	4.02E-02	1.4114	0.4971	NS	NS	1.0014	0.0019827
Cervonic acid	Heart	Positive	7.94E-05	2.58E-03	0.32755	-1.6102	NS	NS	0.93464	-0.097513
Methyl oleoylethanolamide	Heart	Positive	3.89E-07	5.44E-04	0.30528	-1.7118	2.15E-04	NS	0.59437	-0.75057
DELTA.17-U-46619	Heart	Positive	3.67E-02	NS	0.71799	-0.47797	NS	NS	0.93877	-0.091156
PC(22:6/18:0)	Heart	Positive	2.57E-03	2.45E-02	1.3541	0.43735	NS	NS	0.93759	-0.092976
Acetylcarnitine	Heart	Positive	NS	NS	1.3238	0.40464	3.51E-02	NS	0.7238	-0.46634
PC(16:0/22:6)	Heart	Positive	5.41E-03	4.51E-02	1.1827	0.2421	NS	NS	0.93659	-0.094508
Adrenic Acid (22:4, n-6)	Heart	Positive	2.32E-02	NS	0.56321	-0.82825	NS	NS	0.92045	-0.11959
γ-Homolinolenic acid	Heart	Positive	3.87E-04	6.27E-03	0.52484	-0.93004	NS	NS	0.86201	-0.21423
DL-Norvaline	Heart	Positive	2.02E-02	NS	0.68375	-0.54846	5.63E-03	NS	0.71433	-0.48533
2-AG	Heart	Positive	1.85E-03	1.89E-02	0.34981	-1.5154	NS	NS	0.87715	-0.18911
Eicosadienoic acid	Heart	Positive	2.47E-04	4.61E-03	0.36406	-1.4577	NS	NS	0.81349	-0.2978
LysoPE(16:0)	Heart	Positive	5.53E-03	4.53E-02	0.432	-1.2109	NS	NS	0.68951	-0.53636
Gln	Heart	Positive	2.52E-02	NS	1.5181	0.60222	NS	NS	0.88803	-0.17132
7α,12α-Dihydroxycholest-4-en-3-one	Heart	Positive	8.37E-05	2.60E-03	0.23422	-2.0941	NS	NS	0.86757	-0.20495
Methyl ricinoleate	Heart	Positive	5.91E-04	8.20E-03	0.39619	-1.3357	NS	NS	1.1194	0.16277
Methyl DPA	Heart	Positive	2.11E-03	2.09E-02	0.37005	-1.4342	NS	NS	0.9106	-0.13512
Erucamide	Heart	Positive	1.56E-02	NS	0.65836	-0.60306	NS	NS	0.98585	-0.020563
9(10)-EpOME	Heart	Positive	1.70E-03	1.76E-02	0.52731	-0.92328	4.89E-04	NS	0.61706	-0.69653
N-Arachidonoyl-L-alanine	Heart	Positive	1.07E-04	3.02E-03	0.24252	-2.0438	3.18E-02	NS	0.632	-0.66201
2-Linoleoylglycerol	Heart	Positive	5.98E-05	2.28E-03	0.44597	-1.165	NS	NS	0.79351	-0.33369
PC(16:0/20:4)	Spleen	Negative	1.68E-04	1.74E-03	1.2985	0.3769	1.70E-03	1.08E-02	1.2121	0.27752
PS(16:0/18:1)	Spleen	Negative	2.01E-06	4.94E-05	0.67875	-0.55905	1.86E-04	1.83E-03	0.74331	-0.42797
PC(16:0/18:2)	Spleen	Negative	3.29E-03	1.85E-02	1.2725	0.34772	2.52E-03	1.47E-02	1.2789	0.35487
PS(18:0/20:4)	Spleen	Negative	5.27E-03	2.63E-02	1.1937	0.25539	NS	NS	1.1608	0.21508
PE(16:0/18:2)	Spleen	Negative	2.01E-05	3.18E-04	0.61356	-0.70473	4.74E-02	NS	0.82721	-0.27368
Cervonic acid	Spleen	Negative	NS	NS	0.94012	-0.08908	1.41E-02	NS	1.7704	0.82409
PE(18:0/20:4)	Spleen	Negative	3.71E-03	2.00E-02	0.64323	-0.6366	NS	NS	0.99501	-0.0072137
ω-3 Arachidonic acid	Spleen	Negative	NS	NS	1.3311	0.41259	1.18E-02	4.93E-02	1.8112	0.85694
PS(18:0/18:2)	Spleen	Negative	2.07E-05	3.26E-04	0.74614	-0.42248	NS	NS	0.87768	-0.18823
PE(P-18:0/22:6)	Spleen	Negative	NS	NS	0.83069	-0.26762	5.76E-03	2.78E-02	1.6116	0.6885
PS(16:0/20:4)	Spleen	Negative	8.89E-05	1.06E-03	0.75224	-0.41073	3.92E-05	5.03E-04	0.67253	-0.57232
Glu	Spleen	Negative	8.42E-05	1.02E-03	0.74132	-0.43183	1.27E-05	2.15E-04	0.63469	-0.65587
PS(18:0/22:6)	Spleen	Negative	NS	NS	1.081	0.11232	4.67E-02	NS	1.1478	0.19883

PE(16:0/20:4)	Spleen	Negative	2.70E-05	4.01E-04	0.72991	↓	-0.4542	2.22E-04	2.12E-03	0.79107	↓	-0.33812
Asp	Spleen	Negative	2.72E-02	NS	0.83364	↓	-0.26251	1.38E-05	2.25E-04	0.60256	↓	-0.73083
PE(P-18:0/22:6)	Spleen	Negative	7.08E-05	9.06E-04	0.4727	↓	-1.081	NS	NS	0.72367	↓	-0.4666
Mannose 6-Phosphate	Spleen	Negative	1.26E-02	NS	0.77305	↓	-0.37137	1.67E-02	NS	0.78248	↓	-0.35387
GLR	Spleen	Positive	2.70E-03	1.90E-02	1.3355	↑	0.41738	1.68E-03	1.31E-02	1.4569	↑	0.54293
PC(18:0/22:6)	Spleen	Positive	NS	NS	1.0089	↑	0.012813	2.04E-02	NS	0.88795	↓	-0.17145
Hypoxanthine	Spleen	Positive	1.15E-04	1.88E-03	0.58217	↓	-0.7805	6.34E-07	1.62E-05	0.50178	↓	-0.99489
PC(16:1/16:1)	Spleen	Positive	1.75E-09	6.75E-07	0.63929	↓	-0.64545	1.12E-08	6.46E-07	0.62086	↓	-0.68767
LysoPC(17:0)	Spleen	Positive	4.28E-02	NS	0.75044	↓	-0.4142	NS	NS	0.99466	↓	-0.0077273
N-Ac-Phe	Spleen	Positive	5.69E-03	3.18E-02	1.3291	↑	0.41041	NS	NS	1.1312	↑	0.17791
LysoPE(16:0)	Spleen	Positive	6.75E-04	7.46E-03	0.68664	↓	-0.54237	NS	NS	1.1791	↑	0.23769
PC(14:0/16:0)	Spleen	Positive	7.57E-05	1.34E-03	0.62695	↓	-0.67359	1.06E-04	1.23E-03	0.7469	↓	-0.42102
11-HEDE	Spleen	Positive	NS	NS	1.3256	↑	0.40661	1.01E-02	NS	1.8189	↑	0.86304
PC(18:0/18:1)□	Spleen	Positive	1.57E-02	NS	1.152	↑	0.20418	NS	NS	0.91465	↓	-0.12871
L-Valine	Spleen	Positive	9.29E-07	4.93E-05	0.58216	↓	-0.7805	1.64E-09	1.21E-07	0.47058	↓	-1.0875
Arachidonic acid	Spleen	Positive	NS	NS	1.4092	↑	0.49487	3.81E-03	2.59E-02	1.7899	↑	0.83984
Taurolite	Spleen	Positive	3.84E-03	2.42E-02	0.63292	↓	-0.6599	NS	NS	1.3122	↑	0.39194
DCHA-PAF	Spleen	Positive	1.48E-05	3.95E-04	0.79423	↓	-0.33237	7.03E-09	4.51E-07	0.71489	↓	-0.48421
LysoPC(22:0)	Spleen	Positive	NS	NS	0.92673	↓	-0.10978	NS	NS	1.0466	↑	0.065654
PC(18:1/14:0)	Spleen	Positive	2.46E-03	1.81E-02	0.85126	↓	-0.23232	5.38E-06	9.40E-05	0.77067	↓	-0.37581
SM(d18:1/18:1)	Spleen	Positive	4.78E-05	9.38E-04	1.3619	↑	0.44565	2.18E-05	3.18E-04	1.32	↑	0.40051
GSSG	Spleen	Positive	2.38E-02	NS	0.60964	↓	-0.71397	1.59E-03	1.26E-02	0.47616	↓	-1.0705
SM(d18:1/18:0)	Spleen	Positive	NS	NS	1.154	↑	0.20658	3.72E-02	NS	1.1948	↑	0.25678
PC(P-18:0/0:0)	Spleen	Positive	2.54E-06	1.04E-04	0.37062	↓	-1.432	1.33E-04	1.46E-03	0.34645	↓	-1.5293
Arg	Spleen	Positive	1.01E-06	5.10E-05	1.8313	↑	0.87288	2.29E-05	3.26E-04	1.7485	↑	0.80608
3-Indolyllactic acid	Spleen	Positive	1.44E-05	3.89E-04	0.61113	↓	-0.71044	1.90E-06	3.88E-05	0.63671	↓	-0.6513
Glu	Kidney	Negative	NS	NS	0.97058	↓	-0.043084	1.03E-06	1.65E-04	0.80399	↓	-0.31476
2-Hydroxypalmitic acid	Kidney	Negative	2.75E-02	NS	0.78839	↓	-0.34301	NS	NS	1.0588	↑	0.082458
Citric Acid	Kidney	Negative	NS	NS	0.57417	↓	-0.80044	1.78E-02	NS	2.6207	↑	1.3899
Cervonic acid	Kidney	Negative	NS	NS	0.93407	↓	-0.098398	1.32E-02	NS	1.354	↑	0.43726
LysoPE(16:0)	Kidney	Negative	NS	NS	0.90602	↓	-0.14239	3.08E-04	6.50E-03	1.4798	↑	0.56538
PE(P-18:0/22:6)	Kidney	Negative	NS	NS	1.0761	↑	0.10579	3.66E-03	3.45E-02	1.6061	↑	0.68357
PS(18:0/22:6)	Kidney	Negative	3.42E-02	NS	0.87227	↓	-0.19716	NS	NS	0.91973	↓	-0.12071
Phenaceturic acid	Kidney	Negative	3.56E-02	NS	1.6147	↑	0.69123	9.40E-03	NS	4.0261	↑	2.0094
Asp	Kidney	Negative	NS	NS	0.92302	↓	-0.11557	2.19E-02	NS	0.8859	↓	-0.17478
Carbocyclic thromboxane A2	Kidney	Negative	1.99E-03	NS	0.55164	↓	-0.8582	1.86E-03	2.16E-02	1.6133	↑	0.69002
PS(18:0/0:0)	Kidney	Negative	NS	NS	1.1147	↑	0.15663	6.99E-07	1.49E-04	3.1595	↑	1.6597
LysoPC(18:0)	Kidney	Negative	2.04E-02	NS	0.74492	↓	-0.42485	NS	NS	0.95544	↓	-0.065766
PC(18:0/18:1)	Kidney	Positive	1.83E-02	NS	1.1309	↑	0.17746	1.09E-03	1.38E-02	1.2546	↑	0.32719
Eicosapentaenoic acid	Kidney	Positive	1.31E-02	NS	0.69474	↓	-0.52546	NS	NS	0.9571	↓	-0.063263
PC(16:1/16:1)	Kidney	Positive	NS	NS	1.0702	↑	0.097882	1.84E-02	NS	0.86814	↓	-0.204
PC(P-18:0/20:4)	Kidney	Positive	NS	NS	0.96158	↓	-0.056528	2.01E-06	1.86E-04	0.62983	↓	-0.66697
Arachidonoyl Thio-PC	Kidney	Positive	NS	NS	1.0747	↑	0.10387	1.14E-02	NS	1.1696	↑	0.22597
PC(O-16:0/22:6)	Kidney	Positive	NS	NS	0.98209	↓	-0.026068	2.24E-06	1.86E-04	0.64166	↓	-0.64012
LysoPC(O-18:0)	Kidney	Positive	NS	NS	0.68534	↓	-0.54512	1.81E-02	NS	1.4744	↑	0.56009

LysoPC(16:0)	Kidney	Positive	NS	NS	0.94716	↓	-0.078316	1.96E-03	1.99E-02	1.2897	↑	0.36706

Note. All metabolite names are validated through tandem MS.

[a] Numbers are FDR adjusted *P* values. NS = not significant (FDR, $P > 0.05$).

Supplementary Table 3. Radiation effects Pathways

Radiation dysregulation pathways

Table 3A

Heart	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
De novo fatty acid biosynthesis	17(23)	8.40E-05	-	-
Fatty acid activation	11(15)	6.72E-04	3(15)	3.45E-02
Arachidonic acid metabolism	7(9)	3.61E-03	-	-
Leukotriene metabolism	7(9)	3.61E-03	3(9)	6.89E-03
Omega-3 fatty acid metabolism	-	-	2(4)	8.65E-03
Fatty Acid Metabolism	6(8)	8.82E-03	-	-
Limonene and pinene degradation	7(10)	8.91E-03	-	-
Bile acid biosynthesis	-	-	4(17)	9.41E-03
Linoleate metabolism	-	-	3(12)	1.66E-02
Saturated fatty acids beta-oxidation	4(5)	1.75E-02	-	-
Xenobiotics metabolism	4(5)	1.75E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Table 3B

Spleen	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Tyrosine metabolism	12(16)	8.40E-05	-	-
Pyrimidine metabolism	3(3)	9.24E-03	14(16)	5.04E-04
Glycine, serine, alanine and threonine metabolism	9(14)	3.32E-02	12(14)	1.51E-03
Glycerophospholipid metabolism	-	-	15(19)	2.02E-03
Fructose and mannose metabolism	6(6)	2.27E-03	5(6)	4.92E-02
Beta-Alanine metabolism	6(6)	2.27E-03	6(6)	7.06E-03
Glycolysis and Gluconeogenesis	4(4)	2.35E-03	7(7)	3.36E-03
Alanine and Aspartate Metabolism	6(7)	8.91E-03	7(7)	3.36E-03
Vitamin B9 (folate) metabolism	-	-	7(7)	3.36E-03
Aspartate and asparagine metabolism	5(7)	1.36E-02	11(13)	3.70E-03
Urea cycle/amino group metabolism	5(6)	4.20E-03	8(10)	2.12E-02
Vitamin B3 (nicotinate and nicotinamide) metabolism	-	-	6(6)	7.06E-03
Pentose phosphate pathway	-	-	8(9)	7.48E-03
Valine, leucine and isoleucine degradation	3(3)	9.24E-03	3(3)	1.62E-02
Aminosugars metabolism	3(3)	9.24E-03	3(3)	1.62E-02
Lysine metabolism	3(3)	9.24E-03	3(3)	1.62E-02
Tryptophan metabolism	7(9)	1.18E-02	7(9)	3.66E-02
TCA cycle	4(4)	1.31E-02	4(4)	3.00E-02
Carbon fixation	-	-	5(5)	1.43E-02
Glycosphingolipid biosynthesis - globoseries	-	-	5(5)	1.43E-02
Fatty acid activation	-	-	5(7)	2.21E-02
Methionine and cysteine metabolism	4(6)	3.71E-02	9(12)	2.69E-02
Butanoate metabolism	2(2)	3.68E-02	6(7)	2.71E-02

Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	6(7)	2.71E-02
Glutamate metabolism	3(4)	3.94E-02	6(7)	2.71E-02
Galactose metabolism	-	-	6(7)	2.71E-02
Glycosphingolipid biosynthesis - neolactoseries	-	-	4(4)	3.00E-02
Keratan sulfate biosynthesis	-	-	4(4)	3.00E-02
O-Glycan biosynthesis	-	-	4(4)	3.00E-02
Propanoate metabolism	-	-	4(4)	3.00E-02
Glycosphingolipid biosynthesis - lactoseries	-	-	4(4)	3.00E-02
Blood Group Biosynthesis	-	-	4(4)	3.00E-02
Sialic acid metabolism	-	-	7(9)	3.66E-02
N-Glycan biosynthesis	2(2)	3.68E-02	7(9)	3.66E-02
Arginine and Proline Metabolism	2(2)	3.68E-02	-	-
Glutathione Metabolism	-	-	5(6)	4.92E-02

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Table 3C

Kidney	**SD 4**		**SD 9**	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Alanine and Aspartate Metabolism	6(7)	1.68E-04	5(7)	3.42E-02
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	8(8)	4.20E-04
Aspartate and asparagine metabolism	8(15)	1.34E-03	-	-
Glycolysis and Gluconeogenesis	5(7)	1.68E-03	6(7)	6.05E-03
De novo fatty acid biosynthesis	4(11)	2.52E-03	-	-
Vitamin A (retinol) metabolism	3(9)	1.09E-02	5(9)	2.77E-03
Purine metabolism	-	-	10(14)	3.53E-03
Vitamin B1 (thiamin) metabolism	3(3)	3.53E-03	-	-
Omega-3 fatty acid metabolism	3(3)	3.53E-03	-	-
Pyruvate Metabolism	-	-	5(5)	3.70E-03
Methionine and cysteine metabolism	-	-	8(11)	7.73E-03
Aminosugars metabolism	5(9)	8.23E-03	-	-
Arginine and Proline Metabolism	5(9)	8.23E-03	6(9)	3.33E-02
Heparan sulfate degradation	-	-	4(4)	9.83E-03
Histidine metabolism	3(4)	1.34E-02	-	-
Butanoate metabolism	5(10)	1.34E-02	-	-
Beta-Alanine metabolism	-	-	5(6)	1.40E-02
Hexose phosphorylation	2(2)	2.13E-02	-	-
Glycerophospholipid metabolism	7(19)	2.57E-02	-	-
Sialic acid metabolism	4(8)	2.59E-02	-	-
Glycine, serine, alanine and threonine metabolism	-	-	8(13)	2.66E-02
Chondroitin sulfate degradation	-	-	3(3)	2.67E-02
Fructose and mannose metabolism	2(3)	4.68E-02	3(3)	2.67E-02
Glyoxylate and Dicarboxylate Metabolism	-	-	3(3)	2.67E-02
Glutathione Metabolism	2(3)	4.68E-02	3(3)	2.67E-02
Vitamin B9 (folate) metabolism	3(5)	2.72E-02	1(1)	4.00E-02

Glutamate metabolism	-	-	4(5)	3.34E-02
Leukotriene metabolism	-	-	2(4)	3.88E-02
Tyrosine metabolism	-	-	12(23)	3.91E-02
Vitamin K metabolism	-	-	1(1)	4.00E-02
Lysine metabolism	3(6)	4.34E-02	-	-
N-Glycan biosynthesis	3(6)	4.34E-02	-	-
Propanoate metabolism	3(6)	4.34E-02	-	-
Alkaloid biosynthesis II	2(3)	4.68E-02	-	-
Tryptophan metabolism	4(10)	4.89E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

SD 4

Heart

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
De novo fatty acid biosynthesis	17	23	8.40E-05	E613,E933,E898,E82,E227,E687,E926,E826,E119,E379,E810,E261,E455,E490,E373,E203,E438	C06427/C06426,C00249,C01530,C00219,C01595,C06429,C06427/C06426,C00712,C00249,C06429,C03242,C00712,C00219,C01530,C03242,C00249,C00219	acid$(5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arachidonic acid; cis-5,8,11,14-Eicosatetraenoic acid$Linoleate; Linoleic acid; (9Z,12Z)-Octadecadienoic acid; 9-cis,12-cis-Octadecadienoate; 9-cis,12-cis-Octadecadienoic acid$(4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoic acid; 4,7,10,13,16,19-Docosahexaenoic acid; Docosahexaen[illegible]
Fatty acid activation	11	15	6.72E-04	E613,E933,E898,E227,E926,E119,E810,E490,E848,E373,E203	C06427/C06426,C00249,C01530,C01595,C06427/C06426,C00249,C03242,C01530,C06423,C03242,C00249	tearic acid$Linoleate; Linoleic acid; (9Z,12Z)-Octadecadienoic acid; 9-cis,12-cis-Octadecadienoate; 9-cis,12-cis-Octadecadienoic acid$(9Z,12Z,15Z)-Octadecatrienoic acid; alpha-Linolenic acid; 9,12,15-Octadecatrienoic acid; Linolenate; alpha-Linolenate/(6Z,9Z,12Z)-Octadecatrienoic acid; 6,9,12-Octadecatrienoic acid; gamma-Linolenic [illegible]
Arachidonic acid metabolism	7	9	0.003613142	E916,E613,E293,E82,E926,E455,E438	leuktrE4,C06427/C06426,C00127,C00219,C06427/C06426,C00219,C00219	ulfide; GSSG; Oxiglutatione; Oxidized glutathione$(5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arachidonic acid; cis-5,8,11,14-Eicosatetraenoic acid$(9Z,12Z,15Z)-Octadecatrienoic acid; alpha-Linolenic acid; 9,12,15-Octadecatrienoic acid; Linolenate; alpha-Linolenate/(6Z,9Z,12Z)-Octadecatrienoic acid; 6,9,12-Octadecatrienoic [illegible]
Leukotriene metabolism	7	9	0.003613142	E82,E191,E438,E559,E455,E228,E374	C00219,CE5947,C00219,CE5946,C00219,CE5926/CE5930/CE2056/CE1447/CE5534/CE5533,CE5946	-Eicosatetraenoic acid$20-COOH-10,11-dihydro-LTB4$(5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arachidonic acid; cis-5,8,11,14-Eicosatetraenoic acid$10,11-dihydro-20-trihydroxy-leukotriene B4$(5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arachidonic acid; cis-5,8,11,14-Eicosatetraenoic acid$//20-dihydroxyleukotri[illegible]
Omega-3 fatty acid metabolism	-	-	-	-	-	-
Fatty Acid Metabolism	6	8	0.008822788	E933,E898,E227,E119,E490,E203	C00249,C01530,C01595,C00249,C01530,C00249	nitate; Cetylic acid$Octadecanoic acid; Stearate; Stearic acid$Linoleate; Linoleic acid; (9Z,12Z)-Octadecadienoic acid; 9-cis,12-cis-Octadecadienoate; 9-cis,12-cis-Octadecadienoic acid$Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid$Octadecanoic acid; Stearate; Stearic acid$Hexadecanoic aci[illegible]
Limonene and pinene degradation	7	10	0.008906815	E649,E255,E950,E3,E463,E389,E146	C11409/C02452/C00964/C02759,C06099/C06078/C00521,C11409/C02452/C00964/C02759,C11409/C02452/C00964/C02759,C06306,C02576,C06099/C06306/C06078/C00521	onene; (+)-(4R)-Limonene//(-)-Limonene; (-)-(S)-Limonene; (-)-(4S)-Limonene$(+)-trans-Carveol; (4S,6R)-trans-Carveol/Perillyl alcohol; (-)-Perillyl alcohol; p-Mentha-1,8-dien-7-ol; (-)-Perillylalcohol/(-)-trans-Carveol/$(+)-trans-Carveol; (4S,6R)-trans-Carveol/Perillyl alcohol; (-)-Perillyl alcohol; p-Mentha-1,8-dien-7-ol; (-)-Perillylal[illegible]
Bile acid biosynthesis	-	-	-	-	-	-
Linoleate metabolism	-	-	-	-	-	-
Saturated fatty acids beta-oxidation	4	5	0.017477523	E801,E119,E933,E203	C02990,C00249,C00249,C00249	L-Palmitoylcarnitine$Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid$Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid$Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid
Xenobiotics metabolism	4	5	0.017477523	E119,E203,E933,E769	C00249,C00249,C00249,C00829	Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid$Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid$Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid$Naphthalene

SD 4

Spleen

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
Tyrosine metabolism	12	16	8.40266E-05	E420,E408,E563,E335,E201,E163,E35,E584,E461,E30,E483,E360	CE4888/C05578,C00355,C05589/C00788,C00025,C00544/C01161/C05577,CE5626,C05583/C05582,C05838/C00166/C02763/C00811,C01183/C02735/C00483,C00127,C00079/CE2172,CE2888	[illegible]
Pyrimidine metabolism	3	3	0.009242921	E335,E569,E127	C00025,C00169,C00092/C05345/C00085/C00103/C01172/C01177/C00636/C03862/C04006/C01097/C01094/C03546/C00446/C00275/CE3075	[illegible]
Glycine, serine, alanine and threonine me	9	14	0.033190488	E18,E686,E141,E366,E501,E303,E395,E58,E547	C00256/C00186/C00184/C01013,C01026/C01205/C02356/C00334/C03284/C05145,C05519/C00188,CE0737/C00546/C00511,C00065/C00740,C00037,C01005/C02532,C00099/C00213/C00133/C00041,C05938/C00217/C00025	[illegible]
Glycerophospholipid metabolism	-	-	-	-	-	-
Fructose and mannose metabolism	6	6	0.002268717	E46,E310,E361,E118,E488,E722	C01231/C05378/C03693/C00665/C01220/C00354/C04063/C04062/C03785,C00577,CE1787,C00092/C02965/C05345/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075,C00661/C00111/C00118 [illegible]	[illegible]
Beta-Alanine metabolism	6	6	0.002268717	E18,E686,E341,E75,E547,E58	C00256/C00186/C00184/C01013,C01026/C01205/C02356/C00334/C03284/C05145,C00049/C00402,C00135,C05938/C00217/C00025,C00099/C00213/C00133/C00041	[illegible]
Glycolysis and Gluconeogenesis	4	4	0.002352743	E569,E127,E178,E511	C00169,C00092/C05345/C00085/C00103/C01172/C01177/C00636/C03862/C04006/C01097/C01094/C03546/C00446/C00275/CE3075,C00248,C00256/C00186/C00184/C01013/C00577	[illegible]
Alanine and Aspartate Metabolism	6	7	0.008906815	E121,E341,E592,E303,E58,E547	C00122,C00049/C00402,C05520/C01045/C01042,C00037,C00099/C00213/C00133/C00041,C05938/C00217/C00025	[illegible]
Vitamin B9 (folate) metabolism	-	-	-	-	-	-
Aspartate and asparagine metabolism	5	7	0.013612301	E335,E569,E513,E159,E30	[illegible]	[illegible]
Urea cycle/amino group metabolism	5	6	0.004201328	E335,E502,E569,E461,E563	[illegible]	[illegible]
Vitamin B3 (nicotinate and nicotinamide)	-	-	-	-	-	-
Pentose phosphate pathway	-	-	-	-	-	-
Valine, leucine and isoleucine degradatio	3	3	0.009242921	E335,E553,E178	[illegible]	[illegible]
Aminosugars metabolism	3	3	0.009242921	E335,E392,E127	[illegible]	[illegible]
Lysine metabolism	3	3	0.009242921	E335,E178,E98	[illegible]	[illegible]
Tryptophan metabolism	7	9	0.011763717	E99,E72,E207,E547,E464,E722,E58	[illegible]	[illegible]
TCA cycle	4	4	0.013108142	E342,E336,E293,E121	[illegible]	[illegible]
Carbon fixation	-	-	-	-	-	-
Glycosphingolipid biosynthesis - globoser	-	-	-	-	-	-
Fatty acid activation	-	-	-	-	-	-
Methionine and cysteine metabolism	4	6	0.037139736	E335,E30,E513,E137	[illegible]	[illegible]
Butanoate metabolism	2	2	0.03680363	E335,E553	[illegible]	[illegible]
Ascorbate (Vitamin C) and Aldarate Metab	-	-	-	-	-	-
Glutamate metabolism	3	4	0.039408453	E335,E30,E569	[illegible]	[illegible]
Galactose metabolism	-	-	-	-	-	-
Glycosphingolipid biosynthesis - neolacto	-	-	-	-	-	-
Keratan sulfate biosynthesis	-	-	-	-	-	-
O-Glycan biosynthesis	-	-	-	-	-	-
Propanoate metabolism	-	-	-	-	-	-
Glycosphingolipid biosynthesis - lactoseri	-	-	-	-	-	-
Blood Group Biosynthesis	-	-	-	-	-	-
Sialic acid metabolism	-	-	-	-	-	-
N-Glycan biosynthesis	2	2	0.03680363	E392,E127	[illegible]	[illegible]
Arginine and Proline Metabolism	2	2	0.03680363	E335,E513	[illegible]	[illegible]
Glutathione Metabolism	-	-	-	-	-	-

SD 4

Kidney

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
Alanine and Aspartate Metabolism	6	7	1.68E-04	E754,E306,E77,E653,E301,E689	[illegible]	[illegible]
Ascorbate (Vitamin C) and Aldarate Metab	-	-	-	-	-	-
Aspartate and asparagine metabolism	8	15	0.001344425	E567,E356,E306,E425,E77,E301,E550,E220	[illegible]	[illegible]
Glycolysis and Gluconeogenesis	5	7	0.001680531	E689,E301,E7,E114,E306	[illegible]	[illegible]
De novo fatty acid biosynthesis	4	11	0.002520797	E171,E245,E177,E251	[illegible]	[illegible]
Vitamin A (retinol) metabolism	3	9	0.010923452	E97,E178,E251	[illegible]	[illegible]
Purine metabolism	-	-	-	-	-	-
Vitamin B1 (thiamin) metabolism	3	3	0.003529115	E363,E301,E689	[illegible]	[illegible]
Omega-3 fatty acid metabolism	3	3	0.003529115	E42,E301,E52	[illegible]	[illegible]
Pyruvate Metabolism	-	-	-	-	-	-
Methionine and cysteine metabolism	-	-	-	-	-	-
Aminosugars metabolism	5	9	0.008234602	E77,E618,E306,E114,E689	[illegible]	[illegible]
Arginine and Proline Metabolism	5	9	0.008234602	E356,E77,E567,E653,E689	[illegible]	[illegible]
Heparan sulfate degradation	-	-	-	-	-	-
Histidine metabolism	3	4	0.013360222	E77,E301,E689	[illegible]	[illegible]
Butanoate metabolism	5	10	0.013444248	E425,E77,E301,E306,E689	[illegible]	[illegible]
Beta-Alanine metabolism	-	-	-	-	-	-
Hexose phosphorylation	2	2	0.021258718	E7,E114	[illegible]	[illegible]
Glycerophospholipid metabolism	7	19	0.025712125	E7,E749,E9,E306,E52,E689,E114	[illegible]	[illegible]
Sialic acid metabolism	4	8	0.025880178	E749,E618,E7,E114	[illegible]	[illegible]
Glycine, serine, alanine and threonine me	-	-	-	-	-	-
Chondroitin sulfate degradation	-	-	-	-	-	-
Fructose and mannose metabolism	2	3	0.04680279	E7,E114	[illegible]	[illegible]
Glyoxylate and Dicarboxylate Metabolism	-	-	-	-	-	-
Glutathione Metabolism	2	3	0.04680279	E77,E567	[illegible]	[illegible]
Vitamin B9 (folate) metabolism	3	5	0.027224603	E77,E454,E754	[illegible]	[illegible]
Glutamate metabolism	-	-	-	-	-	-
Leukotriene metabolism	-	-	-	-	-	-
Tyrosine metabolism	-	-	-	-	-	-
Vitamin K metabolism	-	-	-	-	-	-
Lysine metabolism	3	6	0.043357701	E356,E77,E301	[illegible]	[illegible]
N-Glycan biosynthesis	3	6	0.043357701	E391,E7,E114	[illegible]	[illegible]
Propanoate metabolism	3	6	0.043357701	E425,E301,E689	[illegible]	[illegible]
Alkaloid biosynthesis II	2	3	0.04680279	E393,E301	[illegible]	[illegible]
Tryptophan metabolism	4	10	0.048903453	E77,E301,E7,E409	[illegible]	[illegible]

Heart

SD9

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
De novo fatty acid biosynthesis	-	-	-	-	-	-
Fatty acid activation	3	15	0.0344509	E38,E20,E948	C06426/C06427,C06426/C06427,C00249	[illegible]
Arachidonic acid metabolism	-	-	-	-	-	-
Leukotriene metabolism	3	9	0.0068902	E944,E459,E939	CE5947,CE5533/CE5926/CE5930/CE2056/CE1447/CE5534,CE5946	20-COOH-10,11-dihydro-LTB4$///20-dihydroxyleukotriene B4/11-dehydrothromboxane B2/$10,11-dihydro-20-trihydroxy-leukotriene B4
Omega-3 fatty acid metabolism	2	4	0.0086547	E38,E20	C06426/C06427,C06426/C06427	[illegible]
Fatty Acid Metabolism	-	-	-	-	-	-
Limonene and pinene degradation	-	-	-	-	-	-
Bile acid biosynthesis	4	17	0.009411	E486,E370,E509,E293	C05463/C05465,CE4874/CE1277/CE1278/CE1279,C05455/C01561,C06341/C05458/C05453/C05501/C15518/C15520/CE5530/C05499/C05445	[illegible]
Linoleate metabolism	3	12	0.0165532	E563,E38,E20	C14762/C14825/C14826,C06426/C06427,C06426/C06427	[illegible]
Saturated fatty acids beta-oxidation	-	-	-	-	-	-
Xenobiotics metabolism	-	-	-	-	-	-

Spleen

SD9

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
Tyrosine metabolism	-	-	-	-	-	-
Pyrimidine metabolism	14	16	0.0005042	E169,E223,E353,E207,E274,E23,E140,E180,E689,E470,E608,E67,E168,E537	[illegible]	[illegible]
Glycine, serine, alanine and threonine metabolism	12	14	0.0015125	E307,E207,E123,E140,E86,E252,E223,E274,E608,E672,E125,E353	C00037,C00164/C00109/C00349/C06002/C00232,C00065/C00740,C00143,C05519/C00188,CE0737/C00546/C00511,C00217/C05938/C00025,C00020/C00362,C00099/C00213/C00133/C00041,C01005/C02532,C00256/C00186/C00184/C01013,C05145/C01026/C01205/C02356/C00334/C03284	[illegible]
Glycerophospholipid metabolism	15	19	0.0020166	E495,E638,E460,E397,E123,E5,E180,E23,E261,E196,E251,E117,E125,E282,E445	[illegible]	[illegible]
Fructose and mannose metabolism	5	6	0.0491555	E180,E262,E495,E261,E638	[illegible]	[illegible]
Beta-Alanine metabolism	6	6	0.0070582	E169,E363,E223,E608,E125,E353	C00402/C00049,C00135,C00217/C05938/C00025,C00099/C00213/C00133/C00041,C00256/C00186/C00184/C01013,C05145/C01026/C01205/C02356/C00334/C03284	[illegible]
Glycolysis and Gluconeogenesis	7	7	0.0033611	E495,E180,E84,E261,E274,E125,E262	[illegible]	[illegible]
Alanine and Aspartate Metabolism	7	7	0.0033611	E307,E169,E511,E223,E274,E608,E508	C00037,C00402/C00049,C05520/C01045/C01042,C00217/C05938/C00025,C00020/C00362,C00099/C00213/C00133/C00041,C00122	[illegible]
Vitamin B9 (folate) metabolism	7	7	0.0033611	E307,E21,E123,E511,E140,E223,E189	C00037,C05928,C00065/C00740,C05520/C01045/C01042,C00143,C00217/C05938/C00025,C05928	[illegible]
Aspartate and asparagine metabolism	11	13	0.0036972	E307,E129,E169,E194,E116,E207,E223,E274,E694,E353,E653	C00037,C06001/C01089/C03197/C00989/C05984,C00402/C00049,C04281/C04282/C01879,C02238,C00164/C00109/C00349/C06002/C00232,C00217/C05938/C00025,C00020/C00362,C03287,C05145/C01026/C01205/C02356/C00334/C03284,C00127	[illegible]
Urea cycle/amino group metabolism	8	10	0.0211747	E307,E169,E140,E223,E608,E694,E508,E353	C00037,C00402/C00049,C00143,C00217/C05938/C00025,C00099/C00213/C00133/C00041,C03287,C00122,C05145/C01026/C01205/C02356/C00334/C03284	[illegible]
Vitamin B3 (nicotinate and nicotinamide) metabolism	6	6	0.0070582	E22,E256,E169,E689,E223,E274	C10164/C00253,C01185,C00402/C00049,C01101/C03736/C00442/C00199,C00217/C05938/C00025,C00020/C00362	[illegible]
Pentose phosphate pathway	8	9	0.0074784	E495,E180,E689,E700,E274,E315,E288,E261	[illegible]	[illegible]
Valine, leucine and isoleucine degradation	3	3	0.0162171	E417,E384,E37	C00025,C00248,C00431/C00183/C00719	[illegible]
Aminosugars metabolism	3	3	0.0162171	E417,E486,E385	C00025,C00128,C00092/C05345/C00085/C00103/C01172/C00636/C01177/C03862/C04006/C01097/C01094/C03546/C00446/C00275/CE3075	[illegible]
Lysine metabolism	3	3	0.0162171	E417,E375,E384	C00025,C00318,C00248	[illegible]
Tryptophan metabolism	7	9	0.0366356	E22,E261,E223,E274,E608,E639,E350	C10164/C00253,C00795/C00095/C00267/C00031/C00137/C00738/C00221/C00962/C00247/C01582/C00936/C00159,C02336/C00984/C00293/C00124,C00217/C05938/C00025,C00020/C00362,C00099/C00213/C00133/C00041,C02220,C03824	[illegible]
TCA cycle	4	4	0.0299975	E191,E508,E732,E84	C00042/C02170,C00122,C00311/C00158/C04575,C00149	[illegible]
Carbon fixation	5	5	0.0142845	E180,E315,E169,E495,E262	[illegible]	[illegible]
Glycosphingolipid biosynthesis - globoseries	5	5	0.0142845	E516,E168,E23,E261,E338	[illegible]	[illegible]
Fatty acid activation	5	7	0.022099	E437,E24,E566,E198,E394	adrn,C01530,tettet6,C00712/C01712,C03242	[illegible]
Methionine and cysteine metabolism	9	12	0.0268885	E307,E207,E123,E223,E274,E395,E36,E167,E653	[illegible]	[illegible]
Butanoate metabolism	6	7	0.0271406	E191,E207,E129,E223,E274,E353	[illegible]	[illegible]
Ascorbate (Vitamin C) and Aldarate Metabolism	6	7	0.0271406	E209,E732,E132,E570,E426,E653	C00818,C00311/C00158/C04575,C01620,C02045,C02147,C00127	[illegible]
Glutamate metabolism	6	7	0.0271406	E191,E207,E223,E608,E353,E653	[illegible]	[illegible]
Galactose metabolism	6	7	0.0271406	E495,E638,E180,E261,E168,E262	[illegible]	[illegible]
Glycosphingolipid biosynthesis - neolactoseries	4	4	0.0299975	E338,E168,E516,E23	C00043/C01170/C00203,C00029/C00052,C00128,C00055	[illegible]
Keratan sulfate biosynthesis	4	4	0.0299975	E168,E23,E516,E338	C00029/C00052,C00055,C00128,C00043/C01170/C00203	[illegible]
O-Glycan biosynthesis	4	4	0.0299975	E338,E168,E516,E23	C00043/C01170/C00203,C00029/C00052,C00128,C00055	[illegible]
Propanoate metabolism	4	4	0.0299975	E274,E125,E207,E129	[illegible]	[illegible]
Glycosphingolipid biosynthesis - lactoseries	4	4	0.0299975	E168,E23,E516,E338	C00029/C00052,C00055,C00128,C00043/C01170/C00203	[illegible]
Blood Group Biosynthesis	4	4	0.0299975	E168,E23,E516,E338	C00029/C00052,C00055,C00128,C00043/C01170/C00203	[illegible]
Sialic acid metabolism	7	9	0.0366356	E23,E460,E123,E180,E261,E251,E516	[illegible]	[illegible]
N-Glycan biosynthesis	7	9	0.0366356	E338,E610,E23,E180,E261,E168,E516	[illegible]	[illegible]
Arginine and Proline Metabolism	-	-	-	-		
Glutathione Metabolism	5	6	0.0491555	E608,E653,E307,E223,E194	[illegible]	[illegible]

Kidney

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
Alanine and Aspartate Metabolism	5	7	0.0341988	E483,E3,E487,E28,E54	C00122,C00217/C05938/C00025,C00222/C00022,C00266/C00033,C00049/C00402	[illegible]
Ascorbate (Vitamin C) and Aldarate Metabolism	8	8	4.20E-04	E212,E64,E431,E761,E330,E499,E352,E112	C00818,C02045,glac/C00072/C02670,C00257/C00800,C00618/C06472/C00191,C01620,C00311/C00158/C04575,CE5985	[illegible]
Aspartate and asparagine metabolism	-	-	-	-		
Glycolysis and Gluconeogenesis	6	7	0.0060499	E487,E592,E28,E441,E17,E444	[illegible]	[illegible]
De novo fatty acid biosynthesis	-	-	-	-		
Vitamin A (retinol) metabolism	5	9	0.0027729	E303,E160,E157,E277,E43	C15492,CE5014,CE5757,retinol-cis-13/retinol-cis-11/CE5590/CE1754,C00899/C00473	[illegible]
Purine metabolism	10	14	0.0035291	E493,E36,E431,E53,E3,E487,E575,E483,E54,E670	[illegible]	[illegible]
Vitamin B1 (thiamin) metabolism	-	-	-	-		
Omega-3 fatty acid metabolism	-	-	-	-		
Pyruvate Metabolism	5	5	0.0036972	E444,E487,E367,E17,E28	C00149,C00222/C00022,CE0737/C00546/C00511,C00256/C00186/C00184/C01013,C00266/C00033	[illegible]
Methionine and cysteine metabolism						
Aminosugars metabolism						
Arginine and Proline Metabolism						
Heparan sulfate degradation						
Histidine metabolism						
Butanoate metabolism						
Beta-Alanine metabolism	5	6	0.0140324	E3,E17,E487,E54,E628	[illegible]	[illegible]
Hexose phosphorylation	-	-	-	-		
Glycerophospholipid metabolism	-	-	-	-		
Sialic acid metabolism	-	-	-	-		
Glycine, serine, alanine and threonine metabolism	8	13	0.0265524	E487,E367,E159,E628,E3,E28,E17,E240	[illegible]	[illegible]
Chondroitin sulfate degradation	3	3	0.0267204	E330,E592,E36	[illegible]	[illegible]
Fructose and mannose metabolism	3	3	0.0267204	E441,E115,E592	[illegible]	[illegible]
Glyoxylate and Dicarboxylate Metabolism	3	3	0.0267204	E28,E36,E240	C00266/C00033,C00312/C00310/C00508/C00259/C00181/C00309/C00121,C00258	[illegible]
Glutathione Metabolism	3	3	0.0267204	E3,E109,E52	C00217/C05938/C00025,C00097,C04281/C04282/C01879	[illegible]
Vitamin B9 (folate) metabolism	1	1	0.0399966	E130	C00065/C00740	[illegible]
Glutamate metabolism	4	5	0.0334426	E3,E487,E440,E628	C00217/C05938/C00025,C00222/C00022,C00042/C02170,C05145/C01026/C01205/C02356/C00334/C03284	[illegible]
Leukotriene metabolism	2	4	0.0388203	E132,E247	C00219,CE4995	[illegible]
Tyrosine metabolism	12	23	0.0390723	E163,E487,E311,E334,E331,E517,E109,E316,E431,E3,E397,E483	[illegible]	[illegible]
Vitamin K metabolism	1	1	0.0399966	E134	C02059/C01628	[illegible]
Lysine metabolism	-	-	-	-		
N-Glycan biosynthesis	-	-	-	-		
Propanoate metabolism	-	-	-	-		
Alkaloid biosynthesis II	-	-	-	-		
Tryptophan metabolism	-	-	-	-		

emialdehyde/(S)-Methylmalonate semial
$AMP; Adenosine 5'-monopho
te; D-myo-Inositol 1-phosphate; 1D-myo-Inositol 1-mon

l-monophosphate; Inositol 3-monophosphate; 1L-myo-Inositol 1-phosphate; L-m

emialdehyde/Succinate
butanoate; (S)-3-Amino-isobutyrate; L-

l-monophosphate; Inositol 3-monophosphate; 1L-myo-Inositol 1-phosphate; L-m

D-myo-Inositol 4-phosphate; 1D-myo-Inositol 4-phosphate; 1D-myo-In

onophosphate$beta-Alanine; 3-Ami

-Adenosine monophosphate; Adenos

)-2-Aminobutanoate; (S)-2-Aminobut
hate; myo-Inositol 3-monophosphate; Inositol 3-monophosphate; 1L-myo-Inositol

te$(S)-3-Hydroxyisobutyrate/(R)-3-Hydroxybut

ate; Inositol 3-phosphate; 1D-myo-Inositol 3-monophosphate;
-Inositol 3-monophosphate; myo-Inositol 3-monophosphate; Inositol 3-monoph

hate/alpha-D-Hexose 1-phosphate/b

obutyrate; 4-Aminobutyric acid; gamm

: acid; Glutamate$Glycolaldehyde; Hydrox

myo-Inositol 4-phosphate; D-myo-Inositol 4-phosphate; 1D-myo-Inositol 4-

ate$adrenochrome/Hippurate; Hippuric acid;

Supplementary Table 4. Metabolic Changes due to amifostine treatment (side effects)

TABLE 4A

Amifostine 50mg side effect in SD 4 for validated metabolites across all tissues

Name	Organ/Tissue	*p-value*	*FDR* [a]	*Fold Change*	*Log2(FC)*
PC(16:0/18:2)	Heart	5.16E-04	*NS*	1.2581	0.3313
PC(16:0/20:5)	Heart	1.46E-03	*NS*	1.22	0.28685
Arachidonoyl Thio-PC	Heart	3.06E-03	*NS*	1.2112	0.27642
PC(16:0/18:1)	Heart	9.31E-03	*NS*	1.2973	0.3755
5'-Adenylic acid	Heart	2.01E-02	*NS*	1.6784	0.74711
PC(16:1/16:1)	Heart	3.62E-02	*NS*	1.3142	0.3942
PC(16:0/20:4)	Spleen	4.00E-02	*NS*	1.1496	0.20108
LysoPE(18:0)	Kidney	9.80E-04	*NS*	0.75206	-0.41108
Glu	Kidney	3.64E-03	*NS*	1.1143	0.15609
2-Hydroxypalmitic acid	Kidney	4.13E-03	*NS*	1.4594	0.54533
Citric Acid	Kidney	5.11E-03	*NS*	3.4518	1.7873
PC(16:0/20:4)	Kidney	8.73E-03	*NS*	1.5163	0.60052
PC(16:0/18:2)	Kidney	1.31E-02	*NS*	1.4881	0.57346
Cervonic acid	Kidney	2.44E-02	*NS*	0.77093	-0.37532
PC(16:0/22:6)	Kidney	2.91E-02	*NS*	1.2456	0.3168
PI(18:0/20:4)	Kidney	3.63E-02	*NS*	1.8556	0.8919
PC(18:1/16:0)	Kidney	4.10E-02	*NS*	1.1882	0.24875
LysoPE(16:0)	Kidney	4.31E-02	*NS*	0.86704	-0.20584
14(15)-EpEDE	Kidney	4.91E-02	*NS*	0.78772	-0.34424
PC(18:0/22:6)	Kidney	4.94E-02	*NS*	1.3458	0.42849

Note. All metabolite names are validated through tandem MS.

[a] Numbers are FDR adjusted *P* values. NS = not significant (FDR, *P* value > 0.05).

TABLE 4B

Amifostine 200mg side effect in SD 4 for validated metabolites across all tissues

Name	Organ/Tissue	*p-value*	*FDR* [a]	*Fold Change*	*Log2(FC)*
PC(16:0/18:1)	Heart	5.24E-03	*NS*	1.2747	0.35012
Cer(d18:1/20:0)	Heart	2.98E-02	*NS*	0.47695	-1.0681
PG(16:0/18:1)	Heart	2.83E-02	*NS*	0.51327	-0.96222
PG(18:1/18:1)	Heart	2.08E-02	*NS*	0.55572	-0.84757
LysoPE(18:0)	Kidney	1.03E-03	*NS*	0.82492	-0.27767
Glu	Kidney	3.28E-02	*NS*	1.1272	0.17274
PS(16:0/20:4)	Kidney	2.18E-02	*NS*	0.84246	-0.24732

Note. All metabolite names are validated through tandem MS.

[a] Numbers are FDR adjusted *P* values. NS = not significant (FDR, *P* value > 0.05).

TABLE 4C

Amifostine 50mg side effect in SD 9 for validated metabolites across all tissues

Name	Organ/Tissue	*p-value*	*FDR* [a]	*Fold Change*	*Log2(FC)*
PC(16:0/18:2)	Heart	5.40E-04	*NS*	1.2244	0.29208
Arachidonoyl Thio-PC	Heart	1.41E-02	*NS*	1.1389	0.18765
PC(16:1/16:1)	Heart	2.85E-02	*NS*	1.2215	0.28864
DELTA.17-U-46619	Heart	2.40E-03	*NS*	0.73629	-0.44165
γ-Homolinolenic acid	Heart	4.51E-02	*NS*	0.8078	-0.30792
LysoPC(18:0)	Heart	4.81E-02	*NS*	0.72867	-0.45666
Erucamide	Heart	2.16E-02	*NS*	1.176	0.23391
PC(18:0/18:1)	Heart	3.54E-02	*NS*	1.9092	0.93298
PS(18:0/18:1)	Spleen	1.85E-02	*NS*	1.1983	0.26101
PS(16:0/20:4)	Spleen	3.53E-02	*NS*	0.88142	-0.18211
PE(16:0/20:4)	Spleen	2.33E-02	*NS*	0.89713	-0.15661
PC(14:0/16:0)	Spleen	3.17E-02	*NS*	1.1618	0.21639
LysoPC(22:0)	Spleen	2.43E-02	*NS*	1.0872	0.12057
LysoPE(18:0)	Kidney	3.48E-02	*NS*	0.85927	-0.21882
PC(18:1/16:0)	Kidney	1.18E-02	*NS*	1.1101	0.15064
14(15)-EpEDE	Kidney	1.74E-02	*NS*	0.80136	-0.31947
PS(16:0/20:4)	Kidney	1.27E-02	*NS*	1.1808	0.23982
PC(16:0/18:0)	Kidney	4.91E-02	*NS*	1.1042	0.143
PS(18:0/22:6)	Kidney	1.34E-02	*NS*	1.1979	0.26055
Asp	Kidney	3.58E-03	*NS*	0.81293	-0.2988
Carbocyclic thromboxane A2	Kidney	2.14E-02	*NS*	0.73809	-0.43814
Arachidonic acid	Kidney	1.07E-02	*NS*	0.78308	-0.35276
Arachidonoyl Thio-PC	Kidney	1.40E-02	*NS*	1.0897	0.12395
PC(16:0/20:5)	Kidney	2.41E-02	*NS*	1.0965	0.13285
Phe	Kidney	2.95E-02	*NS*	0.68777	-0.53999

Note. All metabolite names are validated through tandem MS.

[a] Numbers are FDR adjusted *P* values. NS = not significant (FDR, *P* value > 0.05).

TABLE 4D

Amifostine 200mg side effect in SD 9 for validated metabolites across all tissues

Name	Organ/Tissue	*p-value*	*FDR* [a]	*Fold Change*		*Log2(FC)*
PS(18:0/18:1)	Spleen	2.44E-03	*NS*	1.2932	↑	0.37091
PS(18:0/18:2)	Spleen	1.56E-02	*NS*	1.1701	↑	0.2266
PE(16:0/20:4)	Spleen	2.42E-02	*NS*	0.90067	↓	-0.15093
PC(16:0/18:1)	Spleen	1.94E-02	*NS*	0.93569	↓	-0.095905
N-Ac-Phe	Spleen	5.57E-03	*NS*	0.74393	↓	-0.42675
L-Valine	Spleen	2.30E-02	*NS*	0.88045	↓	-0.18369
LysoPC(22:0)	Spleen	4.85E-02	*NS*	1.0959	↑	0.13212
SM(d18:1/18:0)	Spleen	2.46E-02	*NS*	1.2121	↑	0.2775
Arg	Spleen	7.72E-04	*NS*	0.78418	↓	-0.35074
Citric Acid	Kidney	2.05E-02	*NS*	1.7349	↑	0.79481
PC(P-18:0/20:4)	Kidney	9.57E-05	3.76E-02	0.78413	↓	-0.35084
PC(18:1/14:0)	Kidney	3.54E-02	*NS*	1.1501	↑	0.20177
PC(O-16:0/22:6)	Kidney	8.92E-04	*NS*	0.8362	↓	-0.25808

Note. All metabolite names are validated through tandem MS.

[a] Numbers are FDR adjusted *P* values. NS = not significant (FDR, *P* value > 0.05).

TABLE 4E

Amifostine side effect in SD4 and SD9 for validated metabolites across all tissues

				SD4 ami_50/Vehicle				SD4 ami_200/Vehicle				SD9 ami_50/Vehicle				SD9 ami_200/Vehicle			
Matrix	Mode	mz_rt	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
Heart	Positive	758.5699_9.87	PC(16:0/18:2)	5.16E-04	9.35E-01	1.2581	0.3313	2.47E-01	8.07E-01	1.1056	0.14481	5.40E-04	6.07E-01	1.2244	0.29208	7.07E-01	9.98E-01	0.98332	-0.024263
Heart	Positive	780.5537_9.7	PC(16:0/20:5)	1.46E-03	9.35E-01	1.22	0.28685	5.93E-01	9.92E-01	1.049	0.069056	4.60E-01	7.62E-01	1.0451	0.063572	6.52E-01	9.97E-01	0.96989	-0.0441
Heart	Positive	784.5823_9.86	Arachidonoyl Thio-PC	3.06E-03	9.35E-01	1.2112	0.27642	1.89E-01	7.50E-01	1.1192	0.16243	1.41E-02	6.07E-01	1.1389	0.18765	5.80E-01	9.97E-01	0.97134	-0.041954
Heart	Positive	760.5854_9.96	PC(16:0/18:1)	9.31E-03	9.35E-01	1.2973	0.3755	5.24E-03	5.18E-01	1.2747	0.35012	5.79E-01	8.07E-01	1.0391	0.055322	9.44E-02	9.97E-01	0.83565	-0.25903
Heart	Positive	348.0715_0.45	5'-Adenylic acid	2.01E-02	9.35E-01	1.6784	0.74711	1.46E-01	6.88E-01	1.3899	0.47497	1.62E-01	6.14E-01	0.77276	-0.3719	2.90E-01	9.97E-01	0.83727	-0.25623
Heart	Positive	730.5382_9.74	PC(16:1/16:1)	3.62E-02	9.35E-01	1.3142	0.3942	2.60E-01	8.27E-01	1.1554	0.2084	2.85E-02	6.07E-01	1.2215	0.28864	2.60E-01	9.97E-01	0.94585	-0.080312
Heart	Positive	792.5703_9.89	PE(18:0/22:6)	6.91E-02	9.35E-01	1.2064	0.27066	1.65E-01	7.22E-01	1.1611	0.21554	5.65E-01	7.98E-01	1.0642	0.089767	2.42E-01	9.97E-01	0.8794	-0.1854
Heart	Positive	762.5126_9.67	PC(16:0/18:0)	1.07E-01	9.35E-01	1.1988	0.26157	3.03E-01	8.76E-01	1.1218	0.16576	5.29E-01	7.87E-01	0.9441	-0.082987	3.24E-01	9.97E-01	0.90227	-0.14837
Heart	Positive	329.2477_7.48	Cervonic acid	1.11E-01	9.35E-01	0.68047	-0.55541	2.42E-01	8.06E-01	0.76975	-0.37754	9.61E-01	9.85E-01	1.0436	0.061564	1.82E-01	9.97E-01	1.299	0.37744
Heart	Positive	323.2528_8.15	Methyl oleoylethanolamide	1.34E-01	9.35E-01	0.77541	-0.36698	5.87E-02	5.51E-01	0.6974	-0.51995	1.07E-01	6.07E-01	0.8618	-0.21458	5.64E-01	9.97E-01	1.2331	0.30234
Heart	Positive	331.2637_8.11	DELTA.17-U-46619	1.58E-01	9.35E-01	0.83772	-0.25546	3.04E-01	8.76E-01	0.87018	-0.20062	2.40E-03	6.07E-01	0.73629	-0.44165	4.77E-01	9.97E-01	0.94134	-0.087213
Heart	Positive	137.047_0.47	Hypoxanthine	1.65E-01	9.35E-01	0.91312	-0.13113	6.89E-01	9.92E-01	0.97225	-0.040602	8.04E-01	9.10E-01	1.0226	0.032244	5.45E-01	9.97E-01	1.0548	0.076954
Heart	Positive	482.3248_7.43	LysoPE(18:0)	1.78E-01	9.35E-01	1.2461	0.31739	1.36E-01	6.71E-01	1.3886	0.47366	1.83E-01	6.17E-01	0.79026	-0.3396	6.07E-02	9.97E-01	0.69171	-0.53177
Heart	Positive	575.5029_10.8	Cer(d18:1/20:0)	2.18E-01	9.35E-01	0.64473	-0.63323	2.98E-02	5.18E-01	0.47695	-1.0681	9.40E-01	9.73E-01	1.2587	0.33193	2.64E-01	9.97E-01	1.2511	0.32316
Heart	Positive	771.5146_11.04	PG(16:0/18:1)	2.26E-01	9.35E-01	0.692	-0.53116	2.83E-02	5.18E-01	0.51327	-0.96222	7.15E-01	8.74E-01	1.4849	0.57036	1.51E-01	9.97E-01	1.5267	0.61039
Heart	Positive	797.5311_11.06	PG(18:1/18:1)	2.39E-01	9.35E-01	0.75435	-0.40669	2.08E-02	5.18E-01	0.55572	-0.84757	5.56E-01	7.97E-01	1.5086	0.59319	3.53E-01	9.97E-01	1.3023	0.38109
Heart	Positive	834.6007_9.89	PC(22:6/18:0)	2.63E-01	9.35E-01	1.1077	0.14759	6.22E-01	9.92E-01	1.0556	0.078041	8.79E-01	9.40E-01	1.0201	0.028768	1.98E-01	9.97E-01	0.89432	-0.16114
Heart	Positive	342.203_9.11	Methyl DHA	2.72E-01	9.35E-01	0.88443	-0.17719	7.87E-01	9.92E-01	1.0133	0.019082	8.29E-01	9.18E-01	1.0207	0.029514	7.25E-01	9.98E-01	0.95388	-0.068123
Heart	Positive	991.6712_6.71	LysoPC(16:0)	2.89E-01	9.35E-01	1.5493	0.63159	3.03E-01	8.76E-01	1.4619	0.54782	1.09E-01	6.07E-01	0.57649	-0.79463	6.63E-01	9.98E-01	1.1085	0.1486
Heart	Positive	357.2772_8.9	Monoolein	3.49E-01	9.37E-01	0.62002	-0.6896	5.81E-01	9.92E-01	1.2685	0.3431	4.99E-01	7.76E-01	0.73636	-0.44152	9.52E-01	9.98E-01	1.0012	0.0017887
Heart	Positive	204.1241_0.44	Acetylcarnitine	3.53E-01	9.37E-01	1.1591	0.21294	9.99E-01	1.00E+00	1.0387	0.054815	1.78E-01	6.17E-01	0.84473	-0.24343	6.43E-01	9.97E-01	1.0002	0.00031755
Heart	Positive	793.5039_11.59	PG(18:2)	3.54E-01	9.37E-01	0.87509	-0.1925	2.42E-01	8.06E-01	0.84751	-0.23869	6.66E-01	8.50E-01	1.3006	0.3792	2.29E-01	9.97E-01	1.3558	0.43918
Heart	Positive	806.5694_9.78	PC(16:0/22:6)	3.56E-01	9.37E-01	1.0462	0.065137	9.41E-01	9.92E-01	1.0049	0.0070508	7.26E-01	8.78E-01	1.0292	0.041546	2.81E-01	9.97E-01	0.93958	-0.089915
Heart	Positive	333.2791_8.5	Adrenic Acid (22:4, n-6)	3.94E-01	9.44E-01	1.2249	0.2927	6.45E-01	9.92E-01	1.176	0.2339	6.89E-02	6.07E-01	0.77551	-0.36678	8.46E-01	9.98E-01	1.0489	0.068906
Heart	Positive	148.0049_0.43	Glu	4.10E-01	9.44E-01	1.0425	0.059994	7.91E-01	9.92E-01	1.0115	0.016534	9.87E-02	6.07E-01	0.93105	-0.10307	6.15E-01	9.97E-01	0.98348	-0.02403
Heart	Positive	307.2588_8.32	γ-Homolinolenic acid	4.69E-01	9.54E-01	0.88004	-0.18436	8.47E-01	9.92E-01	0.97687	-0.033755	4.51E-02	6.07E-01	0.8078	-0.30792	9.60E-01	9.98E-01	1.0428	0.060452
Heart	Positive	118.0874_0.43	DL-Norvaline	5.05E-01	9.54E-01	1.0537	0.07548	8.22E-01	9.92E-01	0.93975	-0.089652	2.51E-01	6.22E-01	1.1254	0.17049	1.50E-01	9.97E-01	1.1501	0.2017
Heart	Positive	287.2357_8.02	N-Arachidonoyl-L-serine	5.27E-01	9.54E-01	0.94674	-0.078955	8.03E-01	9.92E-01	0.99491	-0.0073657	2.15E-01	6.22E-01	0.85299	-0.2294	4.70E-01	9.97E-01	0.91992	-0.12041
Heart	Positive	379.2825_8.14	2-AG	5.50E-01	9.55E-01	1.2014	0.26473	8.77E-01	9.92E-01	0.98246	-0.02553	9.56E-01	9.82E-01	1.0585	0.081988	2.39E-01	9.97E-01	1.3179	0.39827
Heart	Positive	291.2665_8.27	Eicosadienoic acid	5.92E-01	9.55E-01	0.83194	-0.26545	8.24E-01	9.92E-01	0.94069	-0.088213	5.53E-01	7.95E-01	0.92196	-0.11722	8.86E-01	9.98E-01	1.1031	0.14152
Heart	Positive	454.3896_6.9	LysoPE(16:0)	6.02E-01	9.55E-01	1.3115	0.39126	8.99E-01	9.92E-01	1.1871	0.24748	5.93E-01	8.15E-01	1.2646	0.33864	4.60E-01	9.97E-01	1.2728	0.34803
Heart	Positive	147.0776_0.44	Gln	6.18E-01	9.55E-01	1.0568	0.079707	9.90E-01	9.99E-01	0.97741	-0.032958	1.54E-01	6.12E-01	0.83081	-0.2674	6.52E-01	9.97E-01	1.0521	0.073315
Heart	Positive	162.1136_0.41	L-Carnitine	6.86E-01	9.57E-01	0.96072	-0.057816	4.87E-01	9.84E-01	1.0913	0.12609	5.50E-01	7.95E-01	1.066	0.092172	6.28E-02	9.97E-01	1.2444	0.31542
Heart	Positive	524.3713_7.46	LysoPC(18:0)	6.97E-01	9.57E-01	1.0648	0.090599	1.93E-01	7.56E-01	1.1767	0.23472	4.81E-02	6.07E-01	0.72867	-0.45666	2.83E-01	9.97E-01	0.88169	-0.18166
Heart	Positive	400.2676_7.69	7α,12α-Dihydroxycholest-4-en-3-one	7.09E-01	9.57E-01	0.99648	-0.005088	3.36E-01	9.06E-01	0.77863	-0.361	8.95E-01	9.50E-01	1.0957	0.13187	2.38E-01	9.97E-01	1.4677	0.55358
Heart	Positive	305.2484_8.02	Arachidonic acid	7.13E-01	9.57E-01	0.96396	-0.052951	7.42E-01	9.92E-01	0.9745	-0.037267	1.67E-01	6.17E-01	0.86114	-0.21568	3.98E-01	9.97E-01	0.91735	-0.12446
Heart	Positive	132.0778_0.42	Creatine	7.26E-01	9.57E-01	1.0272	0.038706	8.12E-01	9.92E-01	1.0234	0.033331	1.74E-01	6.17E-01	0.8643	-0.21039	8.24E-01	9.98E-01	1.03	0.042586
Heart	Positive	313.2739_8.01	Methyl ricinoleate	7.56E-01	9.61E-01	0.91811	-0.12326	8.02E-01	9.92E-01	0.9081	-0.13908	2.96E-01	6.42E-01	1.134	0.18136	9.13E-01	9.98E-01	1.1004	0.13808
Heart	Positive	344.2587_8.67	Methyl DPA	7.82E-01	9.62E-01	0.87658	-0.19003	5.80E-01	9.92E-01	0.82852	-0.2714	6.26E-01	8.29E-01	0.93951	-0.090015	2.92E-01	9.97E-01	1.2519	0.32414
Heart	Positive	338.1829_8.61	Erucamide	7.88E-01	9.62E-01	1.0194	0.027651	6.43E-01	9.92E-01	0.92871	-0.10671	2.16E-02	6.07E-01	1.176	0.23391	6.92E-02	9.97E-01	1.186	0.24608
Heart	Positive	279.2321_7.69	9(10)-EpOME	8.02E-01	9.65E-01	0.9603	-0.058443	8.46E-01	9.92E-01	0.95757	-0.062557	5.26E-01	7.87E-01	0.94477	-0.081961	6.56E-01	9.98E-01	1.0568	0.079752
Heart	Positive	375.2612_7.63	N-Arachidonoyl-L-alanine	8.36E-01	9.70E-01	1.1093	0.1496	6.67E-01	9.92E-01	0.94526	-0.081211	8.42E-01	9.23E-01	1.0487	0.068621	5.67E-01	9.97E-01	1.1642	0.21937
Heart	Positive	810.5073_9.69	PC(18:0/18:1)	9.17E-01	9.94E-01	0.97265	-0.040008	3.13E-01	8.84E-01	0.83683	-0.257	3.54E-02	6.07E-01	1.9092	0.93298	7.87E-01	9.98E-01	1.0427	0.060337
Heart	Positive	355.2837_7.63	2-Linoleoylglycerol	9.88E-01	9.98E-01	1.044	0.062064	7.37E-01	9.92E-01	1.0242	0.03453	4.19E-01	7.40E-01	1.1393	0.18809	3.67E-01	9.97E-01	1.2483	0.32
Heart	Positive	353.2668_8.12	15,19-Hhydroxy PGE1	9.98E-01	9.99E-01	0.99532	-0.0067726	4.73E-01	9.77E-01	0.81961	-0.28698	1.64E-01	6.16E-01	1.171	0.22771	6.76E-02	9.97E-01	1.241	0.31147
Spleen	Negative	826.5609_10.2	PC(16:0/20:4)	4.00E-02	8.19E-01	1.1496	0.20108	3.12E-01	1.00E+00	1.0601	0.084258	6.02E-01	9.96E-01	0.96829	-0.046485	4.61E-01	7.91E-01	1.0451	0.063577
Spleen	Negative	760.5127_11.91	PS(16:0/18:1)	5.69E-02	8.19E-01	1.1077	0.14763	1.23E-01	1.00E+00	1.086	0.11902	7.31E-02	9.95E-01	1.0924	0.12748	5.79E-02	5.97E-01	1.1237	0.16828
Spleen	Negative	802.5608_10.24	PC(16:0/18:2)	8.61E-02	8.19E-01	1.1899	0.25082	6.17E-01	1.00E+00	1.0429	0.060614	3.67E-01	9.96E-01	0.93715	-0.093643	7.69E-01	9.19E-01	1.0185	0.026506
Spleen	Negative	810.5295_11.91	PS(18:0/20:4)	2.53E-01	8.19E-01	1.0591	0.08279	5.45E-01	1.00E+00	1.0361	0.0512	2.78E-01	9.96E-01	1.0523	0.07353	2.79E-01	6.93E-01	1.0505	0.07108
Spleen	Negative	788.5428_11.9	PS(18:0/18:1)	2.58E-01	8.19E-01	1.111	0.15186	9.56E-01	1.00E+00	0.9971	-0.0041913	1.85E-02	9.68E-01	1.1983	0.26101	2.44E-03	4.34E-01	1.2932	0.37091
Spleen	Negative	714.5079_10.31	PE(16:0/18:2)	3.53E-01	8.19E-01	0.91791	-0.12357	1.53E-01	1.00E+00	0.87601	-0.19097	2.08E-01	9.96E-01	0.89293	-0.16338	2.38E-01	6.80E-01	0.90439	-0.14498
Spleen	Negative	327.2322_8.65	Cervonic acid	4.25E-01	8.19E-01	0.80024	-0.32149	7.95E-01	1.00E+00	0.84705	-0.23948	6.52E-01	9.96E-01	1.0931	0.12841	3.63E-01	7.33E-01	0.82357	-0.28004
Spleen	Negative	520.2662_7.46	PE(18:0/20:4)	4.43E-01	8.20E-01	0.90123	-0.15003	8.86E-01	1.00E+00	0.97777	-0.032427	9.22E-01	9.96E-01	1.0102	0.014658	2.60E-01	6.88E-01	0.89999	-0.15202
Spleen	Negative	303.2321_8.8	ω-3 Arachidonic acid	4.67E-01	8.28E-01	0.78929	-0.34136	7.89E-01	1.00E+00	1.0294	0.04177	8.28E-01	9.96E-01	0.97082	-0.042722	5.21E-01	8.16E-01	0.90363	-0.14619
Spleen	Negative	786.5289_11.91	PS(18:0/18:2)	5.15E-01	8.36E-01	1.0331	0.046974	4.61E-01	1.00E+00	1.0498	0.070053	9.41E-02	9.96E-01	1.0987	0.13576	1.56E-02	4.72E-01	1.1701	0.2266
Spleen	Negative	464.3138_8.52	PE(P-18:0/22:6)	6.30E-01	8.62E-01	0.96038	-0.058318	3.62E-01	1.00E+00	0.88221	-0.1808	3.31E-01	9.96E-01	1.1065	0.14605	9.27E-01	9.75E-01	0.98209	-0.026074
Spleen	Negative	295.227_7.22	12(13)-EpOME	6.79E-01	8.74E-01	0.83184	-0.26562	3.76E-01	1.00E+00	0.81363	-0.29755	1.47E-01	9.96E-01	1.4861	0.57148	9.92E-01	9.96E-01	0.7683	-0.38026
Spleen	Negative	782.4981_11.91	PS(16:0/20:4)	6.83E-01	8.74E-01	0.9795	-0.029885	4.02E-01	1.00E+00	1.0534	0.075103	3.53E-02	9.68E-01	0.88142	-0.18211	1.22E-01	6.67E-01	0.92376	-0.11442
Spleen	Negative	146.0449_0.62	Glu	6.91E-01	8.78E-01	1.0319	0.045353	8.60E-01	1.00E+00	0.98822	-0.017098	4.49E-01	9.96E-01	0.96647	-0.049206	9.44E-01	9.82E-01	0.99635	-0.0052703
Spleen	Negative	834.6139_10.43	PS(18:0/22:6)	7.15E-01	8.90E-01	0.98547	-0.02111	1.33E-01	1.00E+00	0.92876	-0.10663	2.91E-01	9.96E-01	1.0774	0.1076	2.83E-01	6.93E-01	1.0979	0.13479
Spleen	Negative	738.5085_10.27	PE(16:0/20:4)	7.52E-01	8.98E-01	0.9865	-0.019614	8.80E-01	1.00E+00	1.0059	0.0084357	2.33E-02	9.68E-01	0.89713	-0.15661	2.42E-02	5.26E-01	0.90067	-0.15093
Spleen	Negative	132.0293_0.62	Asp	7.63E-01	9.01E-01	1.0261	0.037221	6.98E-01	1.00E+00	0.96656	-0.049062	1.84E-01	9.96E-01	0.92845	-0.10711	1.01E-01	6.66E-01	0.93377	-0.098861

Spleen	Negative	464.312_7.87	PE(P-18:0/22:6)	7.92E-01	9.15E-01	1.007	0.010034	7.22E-01	1.00E+00	1.0974	0.13403	7.46E-01	9.96E-01	1.0638	0.089205	8.98E-01	9.65E-01	0.96833	-0.046423
Spleen	Negative	259.0216_0.66	Mannose 6-Phosphate	8.81E-01	9.52E-01	0.99162	-0.012141	5.19E-01	1.00E+00	0.95889	-0.06056	4.22E-01	9.96E-01	0.96006	-0.058808	1.59E-01	6.67E-01	1.0613	0.085895
Spleen	Positive	173.0806_0.85	GLR	1.03E-01	8.05E-01	1.3186	0.39902	2.03E-01	1.00E+00	1.1173	0.16003	6.45E-01	9.19E-01	1.0289	0.041114	3.78E-01	6.43E-01	1.0544	0.076426
Spleen	Positive	760.5845_10.36	PC(16:0/18:1)	1.63E-01	8.05E-01	0.95131	-0.072007	2.16E-01	1.00E+00	0.96703	-0.048365	5.62E-01	9.10E-01	0.98314	-0.024529	1.94E-02	2.36E-01	0.93569	-0.095905
Spleen	Positive	834.5996_10.25	PC(18:0/22:6)	1.63E-01	8.05E-01	0.94283	-0.084926	4.29E-01	1.00E+00	0.97061	-0.043035	2.93E-01	7.76E-01	0.95519	-0.066146	2.59E-01	5.57E-01	0.95832	-0.061414
Spleen	Positive	137.0466_0.7	Hypoxanthine	1.65E-01	8.05E-01	0.8846	-0.17691	6.76E-01	1.00E+00	0.9749	-0.036678	6.94E-01	9.24E-01	1.0312	0.044357	3.05E-01	5.99E-01	0.93249	-0.10084
Spleen	Positive	730.544_10.2	PC(16:1/16:1)	1.67E-01	8.05E-01	0.93346	-0.099333	2.06E-01	1.00E+00	0.9512	-0.07218	5.98E-01	9.10E-01	1.0193	0.027559	1.89E-01	4.95E-01	0.94131	-0.087259
Spleen	Positive	510.355_7.9	LysoPC(17:0)	1.71E-01	8.05E-01	0.83158	-0.26608	8.49E-01	1.00E+00	1.045	0.06354	9.38E-01	9.83E-01	1.005	0.0072156	1.38E-01	4.45E-01	0.84877	-0.23656
Spleen	Positive	165.0544_0.71	N-Ac-Phe	2.42E-01	8.05E-01	0.86745	-0.20515	2.27E-01	1.00E+00	0.86717	-0.20562	5.17E-01	8.97E-01	0.92663	-0.10993	5.57E-03	1.79E-01	0.74393	-0.42675
Spleen	Positive	476.2791_7.46	LysoPE(16:0)	3.09E-01	8.05E-01	0.89345	-0.16254	2.65E-01	1.00E+00	0.88799	-0.17138	3.65E-01	8.09E-01	1.0696	0.097115	5.88E-01	7.92E-01	0.96557	-0.050545
Spleen	Positive	706.5434_10.3	PC(14:0/16:0)	3.66E-01	8.05E-01	1.1005	0.13822	3.49E-01	1.00E+00	0.9182	-0.12312	3.17E-02	6.16E-01	1.1618	0.21639	1.55E-01	4.60E-01	1.0951	0.13102
Spleen	Positive	307.2567_9.03	11-HEDE	3.70E-01	8.05E-01	0.79869	-0.3243	8.63E-01	1.00E+00	1.0377	0.053411	5.82E-01	9.10E-01	0.92227	-0.11674	1.43E-01	4.49E-01	0.7888	-0.34226
Spleen	Positive	810.6004_10.33	PC(18:0/18:1)?	3.83E-01	8.05E-01	0.96396	-0.052951	6.43E-01	1.00E+00	1.016	0.022857	1.18E-01	6.57E-01	0.92521	-0.11215	6.37E-02	3.41E-01	0.92758	-0.10846
Spleen	Positive	118.0867_0.67	L-Valine	4.39E-01	8.05E-01	0.94248	-0.085473	1.62E-01	1.00E+00	0.91497	-0.1282	8.26E-01	9.63E-01	0.9848	-0.0221	2.30E-02	2.54E-01	0.88045	-0.18369
Spleen	Positive	305.2477_8.8	Arachidonic acid	4.84E-01	8.05E-01	0.85912	-0.21907	7.66E-01	1.00E+00	1.051	0.071748	6.01E-01	9.10E-01	0.93903	-0.090763	3.13E-01	6.05E-01	0.85615	-0.22407
Spleen	Positive	482.324_8.33	Taurolite	4.93E-01	8.09E-01	0.94309	-0.084539	2.18E-01	1.00E+00	0.85035	-0.23387	8.17E-02	6.46E-01	1.1687	0.2249	4.39E-01	6.92E-01	0.93822	-0.092003
Spleen	Positive	792.5738_10.28	DCHA-PAF	5.51E-01	8.31E-01	0.97663	-0.034116	3.20E-01	1.00E+00	0.96288	-0.054577	1.26E-01	6.68E-01	1.0581	0.081468	6.45E-02	3.43E-01	1.0457	0.064516
Spleen	Positive	580.3577_9.64	LysoPC(22:0)	5.62E-01	8.31E-01	0.96384	-0.05313	4.93E-01	1.00E+00	1.0751	0.10443	2.43E-02	6.16E-01	1.0872	0.12057	4.85E-02	3.17E-01	1.0959	0.13212
Spleen	Positive	732.5571_10.3	PC(18:1/14:0)	5.83E-01	8.43E-01	0.97668	-0.034039	6.46E-01	1.00E+00	0.98262	-0.025287	2.30E-01	7.49E-01	0.95258	-0.070092	1.01E-01	4.04E-01	0.94025	-0.088883
Spleen	Positive	729.5727_10.38	SM(d18:1/18:1)	5.87E-01	8.43E-01	0.97548	-0.035822	7.84E-01	1.00E+00	0.989	-0.015953	1.02E-01	6.48E-01	1.0775	0.10772	5.19E-02	3.27E-01	1.0916	0.1265
Spleen	Positive	613.1586_0.69	GSSG	6.01E-01	8.43E-01	0.92028	-0.11985	7.83E-01	1.00E+00	1.0279	0.039682	7.63E-01	9.48E-01	0.96174	-0.056278	5.35E-01	7.57E-01	0.91626	-0.12618
Spleen	Positive	731.5945_10.43	SM(d18:1/18:0)	6.35E-01	8.57E-01	1.0451	0.063611	7.65E-01	1.00E+00	0.95383	-0.068201	2.87E-01	7.73E-01	1.1122	0.15337	2.46E-02	2.55E-01	1.2121	0.2775
Spleen	Positive	508.372_7.89	PC(P-18:0/0:0)	6.65E-01	8.69E-01	0.97003	-0.043899	8.68E-01	1.00E+00	1.1099	0.15045	8.77E-01	9.72E-01	1.0332	0.047172	5.51E-01	7.69E-01	0.92433	-0.11352
Spleen	Positive	175.0747_0.63	Arg	7.74E-01	9.17E-01	0.99096	-0.013101	1.72E-01	1.00E+00	0.8922	-0.16456	8.06E-02	6.46E-01	0.88755	-0.1721	7.72E-04	1.42E-01	0.78418	-0.35074
Spleen	Positive	206.0677_0.64	3-Indolyllactic acid	8.33E-01	9.35E-01	0.98905	-0.015885	6.91E-01	1.00E+00	0.96955	-0.04461	4.89E-01	8.85E-01	1.0493	0.069399	1.83E-01	4.91E-01	0.93719	-0.093594
Kidney	Negative	480.309_8.31	LysoPE(18:0)	9.80E-04	9.60E-02	0.75206	-0.41108	1.03E-03	2.45E-01	0.82492	-0.27767	3.48E-02	2.51E-01	0.85927	-0.21882	8.58E-02	7.47E-01	0.87348	-0.19516
Kidney	Negative	146.045_0.62	Glu	3.64E-03	1.45E-01	1.1143	0.15609	3.28E-02	9.66E-01	1.1272	0.17274	5.35E-01	7.66E-01	0.97287	-0.039683	6.34E-01	9.98E-01	0.98583	-0.020594
Kidney	Negative	271.2269_8.59	2-Hydroxypalmitic acid	4.13E-03	1.49E-01	1.4594	0.54533	2.07E-01	9.66E-01	1.1066	0.14612	8.24E-01	9.30E-01	0.98154	-0.026879	3.84E-01	9.98E-01	1.0736	0.10241
Kidney	Negative	191.0187_0.7	Citric Acid	5.11E-03	1.74E-01	3.4518	1.7873	6.73E-02	9.66E-01	2.3504	1.2329	5.80E-02	3.07E-01	1.4567	0.54274	2.05E-02	4.77E-01	1.7349	0.79481
Kidney	Negative	826.5608_10.2	PC(16:0/20:4)	8.73E-03	2.15E-01	1.5163	0.60052	9.09E-02	9.66E-01	1.2127	0.27821	2.38E-01	5.20E-01	1.0954	0.1315	6.82E-01	9.98E-01	1.0746	0.10382
Kidney	Negative	802.5607_10.25	PC(16:0/18:2)	1.31E-02	2.44E-01	1.4881	0.57346	2.92E-01	9.66E-01	1.1622	0.21686	1.59E-01	4.41E-01	1.1409	0.19022	7.42E-01	9.98E-01	1.101	0.13885
Kidney	Negative	327.232_8.65	Cervonic acid	2.44E-02	2.90E-01	0.77093	-0.37532	3.40E-01	9.66E-01	0.90954	-0.13679	7.86E-02	3.33E-01	0.8488	-0.2365	6.16E-01	9.98E-01	1.0583	0.081769
Kidney	Negative	850.5611_10.15	PC(16:0/22:6)	2.91E-02	2.99E-01	1.2456	0.3168	3.62E-01	9.66E-01	1.0922	0.12719	1.40E-01	4.15E-01	1.0939	0.12949	7.39E-01	9.98E-01	1.0409	0.05787
Kidney	Negative	886.6084_10.37	PI(18:0/20:4)	3.63E-02	3.03E-01	1.8556	0.8919	3.08E-01	9.66E-01	1.27	0.34486	8.07E-01	9.21E-01	0.97019	-0.043657	4.59E-01	9.98E-01	1.0532	0.074831
Kidney	Negative	804.5756_10.35	PC(18:1/16:0)	4.10E-02	3.07E-01	1.1882	0.24875	1.38E-01	9.66E-01	1.1061	0.14549	1.18E-02	1.96E-01	1.1101	0.15064	2.50E-01	9.98E-01	1.0689	0.096158
Kidney	Negative	452.2776_7.48	LysoPE(16:0)	4.31E-02	3.13E-01	0.86704	-0.20584	8.33E-02	9.66E-01	0.91126	-0.13407	1.71E-01	4.56E-01	0.92278	-0.11595	7.52E-01	9.98E-01	0.98397	-0.023318
Kidney	Negative	303.2321_8.79	14(15)-EpEDE	4.91E-02	3.19E-01	0.78772	-0.34424	7.19E-01	9.77E-01	0.96238	-0.055323	1.74E-02	2.19E-01	0.80136	-0.31947	5.59E-01	9.98E-01	0.96071	-0.05782
Kidney	Negative	878.5919_10.26	PC(18:0/22:6)	4.94E-02	3.19E-01	1.3458	0.42849	5.11E-01	9.66E-01	1.0941	0.1298	1.26E-01	4.03E-01	1.1689	0.22519	8.06E-01	9.98E-01	1.0673	0.093964
Kidney	Negative	781.4888_11.91	PS(16:0/20:4)	9.32E-02	3.87E-01	0.86459	-0.20992	2.18E-02	9.66E-01	0.84246	-0.24732	1.27E-02	1.99E-01	1.1808	0.23982	3.15E-01	9.98E-01	1.0794	0.11027
Kidney	Negative	464.3138_8.52	PE(P-18:0/22:6)	1.96E-01	4.85E-01	0.86057	-0.21664	2.00E-01	9.66E-01	0.90063	-0.15099	9.67E-01	9.91E-01	0.98366	-0.02377	6.20E-01	9.98E-01	1.0539	0.075753
Kidney	Negative	790.5385_10.3	PE(18:0/22:6)	2.64E-01	5.35E-01	0.86625	-0.20715	4.66E-01	9.66E-01	0.93951	-0.090027	3.32E-01	6.08E-01	1.0881	0.12176	8.62E-01	9.98E-01	1.0394	0.055701
Kidney	Negative	806.5851_10.39	PC(16:0/18:0)	4.51E-01	6.70E-01	1.0709	0.098806	6.26E-01	9.67E-01	1.0326	0.046301	4.91E-02	2.85E-01	1.1042	0.143	6.07E-01	9.98E-01	1.0277	0.039425
Kidney	Negative	747.5197_10.26	PG(16:0/18:1)	4.90E-01	7.05E-01	0.94616	-0.07985	9.07E-01	9.90E-01	0.99417	-0.008438	1.41E-01	4.15E-01	1.0872	0.12067	4.69E-01	9.98E-01	1.0485	0.068392
Kidney	Negative	834.5288_11.91	PS(18:0/22:6)	4.94E-01	7.08E-01	0.94944	-0.074847	6.10E-01	9.67E-01	0.96447	-0.052194	1.34E-02	2.01E-01	1.1979	0.26055	4.89E-01	9.98E-01	1.0451	0.063578
Kidney	Negative	192.0654_3.15	Phenaceturic acid	5.46E-01	7.49E-01	1.1016	0.13965	4.91E-01	9.66E-01	1.2544	0.32697	3.02E-01	5.82E-01	1.4638	0.54969	9.70E-01	9.98E-01	0.86383	-0.21118
Kidney	Negative	132.0292_0.62	Asp	6.67E-01	8.25E-01	0.97955	-0.029803	9.56E-02	9.66E-01	0.92226	-0.11676	3.58E-03	1.73E-01	0.81293	-0.2988	3.14E-01	9.98E-01	0.95788	-0.062076
Kidney	Negative	810.5296_11.92	PS(18:0/20:4)	6.97E-01	8.43E-01	0.98844	-0.01677	8.19E-01	9.87E-01	0.98962	-0.015055	6.14E-02	3.09E-01	1.1594	0.21332	4.57E-01	9.98E-01	1.0612	0.085754
Kidney	Negative	329.2477_9.03	Carbocyclic thromboxane A2	8.19E-01	9.14E-01	0.9339	-0.098664	2.82E-01	9.66E-01	1.2425	0.31326	2.14E-02	2.30E-01	0.73809	-0.43814	9.46E-01	9.98E-01	1.0718	0.10007
Kidney	Negative	524.2986_12.01	PS(18:0/0:0)	9.20E-01	9.62E-01	0.98215	-0.025982	6.59E-01	9.69E-01	0.95194	-0.071059	2.79E-01	5.61E-01	0.89602	-0.15839	9.22E-01	9.98E-01	1.0033	0.0048172
Kidney	Negative	568.2675_7.42	LysoPC(18:0)	9.72E-01	9.88E-01	0.99276	-0.010481	6.64E-01	9.72E-01	1.058	0.08139	8.47E-01	9.37E-01	0.99837	-0.0023603	1.84E-01	9.65E-01	1.1924	0.25389
Kidney	Positive	782.5704_10.25	PC(18:0/18:1)	8.95E-02	3.85E-01	1.1456	0.19611	5.52E-02	9.98E-01	1.1623	0.21704	2.76E-01	8.23E-01	1.0426	0.060253	6.17E-01	9.10E-01	1.0322	0.045722
Kidney	Positive	303.2307_8.38	Eicosapentaenoic acid	1.17E-01	4.08E-01	0.77409	-0.36943	2.46E-01	9.98E-01	0.84297	-0.24644	6.46E-01	9.43E-01	0.97238	-0.040409	9.94E-01	9.98E-01	1.0239	0.034107
Kidney	Positive	730.545_10.19	PC(16:1/16:1)	1.46E-01	4.24E-01	1.1641	0.21924	1.18E-01	9.98E-01	1.0852	0.11801	7.90E-02	5.60E-01	1.0883	0.12202	7.01E-01	9.20E-01	1.0169	0.024152
Kidney	Positive	305.2473_8.78	Arachidonic acid	1.48E-01	4.26E-01	0.77661	-0.36473	9.51E-01	9.99E-01	0.99592	-0.0059039	1.07E-02	4.04E-01	0.78308	-0.35276	3.38E-01	8.61E-01	0.94236	-0.085644
Kidney	Positive	794.5986_10.27	PC(P-18:0/20:4)	1.77E-01	4.44E-01	0.86766	-0.2048	4.55E-01	9.98E-01	0.93697	-0.093927	1.66E-01	7.31E-01	0.93657	-0.094536	9.57E-05	3.76E-02	0.78413	-0.35084
Kidney	Positive	732.5564_10.31	PC(18:1/14:0)	1.82E-01	4.52E-01	1.2011	0.26431	7.18E-02	9.98E-01	1.17	0.22651	8.50E-02	5.78E-01	1.1036	0.1422	3.54E-02	8.49E-01	1.1501	0.20177
Kidney	Positive	784.5822_10.28	Arachidonoyl Thio-PC	2.43E-01	5.06E-01	1.1155	0.15764	7.82E-02	9.98E-01	1.1302	0.17663	1.40E-02	4.04E-01	1.0897	0.12395	5.11E-01	8.83E-01	1.0416	0.058805
Kidney	Positive	792.59_10.26	PC(O-16:0/22:6)	2.71E-01	5.29E-01	0.90059	-0.15107	4.86E-01	9.98E-01	0.94557	-0.080738	7.06E-01	9.43E-01	0.98607	-0.020245	8.92E-04	7.25E-02	0.8362	-0.25808
Kidney	Positive	510.3542_7.88	LysoPC(O-18:0)	3.46E-01	5.83E-01	0.80998	-0.30403	9.84E-01	9.99E-01	1.0274	0.039053	3.55E-01	8.36E-01	0.90799	-0.13925	5.94E-01	9.09E-01	1.0835	0.11569
Kidney	Positive	780.5565_10.15	PC(16:0/20:5)	4.72E-01	6.64E-01	1.0496	0.069774	9.85E-01	9.99E-01	1.0005	0.00078005	2.41E-02	4.61E-01	1.0965	0.13285	1.56E-01	8.49E-01	1.0547	0.07685
Kidney	Positive	166.0862_1.11	Phe	5.90E-01	7.50E-01	0.92122	-0.11837	9.88E-01	9.99E-01	1.0878	0.12136	2.95E-02	4.78E-01	0.68777	-0.53999	9.25E-01	9.75E-01	0.98175	-0.026569
Kidney	Positive	731.5898_10.4	Sphingomyelin	7.16E-01	8.32E-01	0.96784	-0.047152	8.36E-01	9.99E-01	1.0016	0.0022645	6.51E-01	9.43E-01	1.0348	0.049348	7.91E-01	9.46E-01	1.0231	0.032973
Kidney	Positive	137.0462_0.72	Hypoxanthine	7.41E-01	8.39E-01	0.97365	-0.038532	4.41E-01	9.98E-01	1.0854	0.11823	3.48E-01	8.36E-01	0.95647	-0.064208	5.05E-01	8.83E-01	1.0267	0.037967
Kidney	Positive	123.0415_0.69	Niacinamide	8.51E-01	9.01E-01	0.97975	-0.029519	5.12E-01	9.98E-01	1.0901	0.12451	4.81E-01	8.78E-01	0.96316	-0.054146	1.71E-01	8.49E-01	1.0861	0.1191
Kidney	Positive	518.3202_7.49	LysoPC(16:0)	9.15E-01	9.44E-01	1.0229	0.032597	3.89E-01	9.98E-01	1.1371	0.18538	6.01E-01	9.36E-01	0.96775	-0.047297	1.95E-01	8.49E-01	1.0968	0.13331

TABLE 5

Amifostine protection effect in SD4 and SD9 for validated metabolites across all tissues

			Recovery Effect Indicator				Recovery Effect Indicator II				SD4												SD9											
			SD 4		SD 9		SD 4		SD 9		Radiation				Amifostine 50mg				Amifostine 200mg				Radiation				Amifostine 50mg				Amifostine 200mg			
Name	**Matrix**	**Mode**	**50mg**	**200mg**	**50mg**	**200mg**	**50mg**	**200mg**	**50mg**	**200mg**	***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)***
PC(16:0/18:2)	Heart	Positive	*	-	-	*	x	x	-	-	2.97E-04	5.20E-03	0.7808	-0.3570	1.49E-01	8.09E-01	1.1346	0.1821	6.79E-01	9.85E-01	0.9783	-0.0317	9.80E-01	1.00E+00	1.0147	0.0210	2.85E-02	1.00E+00	1.2006	0.2637	9.37E-01	9.66E-01	0.9834	-0.0241
PC(16:0/20:5)	Heart	Positive	-	-	*	*	-	-	-	-	1.17E-02	7.52E-02	0.8609	-0.2161	5.58E-01	9.96E-01	0.9721	-0.0408	3.07E-01	9.85E-01	0.9466	-0.0791	5.03E-02	9.20E-01	0.8411	-0.2497	4.24E-02	1.00E+00	1.1641	0.2193	2.88E-01	6.80E-01	1.0636	0.0889
Arachidonoyl Thio-PC	Heart	Positive	*	-	-	*	-	-	-	-	1.77E-01	4.61E-01	0.9235	-0.1148	3.35E-01	9.19E-01	1.0842	0.1167	1.20E-02	9.85E-01	0.8672	-0.2057	4.12E-03	3.49E-01	1.2167	0.2830	3.82E-01	1.00E+00	1.0544	0.0764	3.54E-02	6.33E-01	0.8668	-0.2062
PC(16:0/18:1)	Heart	Positive	*	*	-	-	-	-	-	-	3.48E-01	6.40E-01	0.9128	-0.1316	1.01E-01	7.87E-01	1.1058	0.1451	9.89E-01	9.97E-01	1.0068	0.0098	6.77E-01	9.76E-01	1.0251	0.0358	3.91E-02	1.00E+00	1.1558	0.2089	3.11E-01	6.89E-01	1.0584	0.0818
5'-Adenylic acid	Heart	Positive	*	*	*	*	-	-	-	-	1.10E-01	3.48E-01	1.3881	0.4731	1.20E-01	7.91E-01	0.7360	-0.4423	4.27E-01	9.85E-01	0.9070	-0.1408	3.76E-01	9.40E-01	1.1272	0.1727	5.96E-02	1.00E+00	0.7223	-0.4694	4.11E-01	7.02E-01	0.8974	-0.1562
PC(16:1/16:1)	Heart	Positive	*	*	*	-	x	x	-	-	1.34E-03	1.46E-02	0.7520	-0.4113	4.10E-01	9.83E-01	1.1319	0.1788	1.42E-01	9.85E-01	1.1297	0.1760	1.58E-01	9.40E-01	0.8958	-0.1588	7.97E-02	1.00E+00	1.2241	0.2918	5.91E-01	7.82E-01	0.9407	-0.0882
PE(18:0/22:6)	Heart	Positive	*	-	*	*	x	x	-	-	5.45E-04	7.79E-03	1.4382	0.5243	2.59E-01	8.90E-01	0.9326	-0.1006	9.17E-01	9.91E-01	1.0036	0.0052	6.52E-01	9.70E-01	1.0307	0.0436	5.59E-01	1.00E+00	0.9589	-0.0606	4.92E-01	7.27E-01	0.9586	-0.0610
PC(16:0/18:0)	Heart	Positive	*	*	-	*	x	x	-	-	4.71E-03	4.02E-02	1.4114	0.4971	1.34E-01	7.91E-01	0.9255	-0.1117	7.47E-02	9.85E-01	0.9087	-0.1382	9.17E-01	1.00E+00	1.0014	0.0020	4.96E-01	1.00E+00	1.0660	0.0922	8.58E-01	9.30E-01	0.9916	-0.0121
Cervonic acid	Heart	Positive	*	*	-	*	x	x	-	-	7.94E-05	2.58E-03	0.3276	-1.6102	2.95E-01	8.95E-01	1.2547	0.3273	7.90E-01	9.86E-01	1.0342	0.0485	5.74E-01	9.64E-01	0.9346	-0.0975	9.09E-01	1.00E+00	0.9765	-0.0343	1.00E-01	6.38E-01	1.7024	0.7676
Methyl oleoylethanolamide	Heart	Positive	*	*	*	*	x	x	-	-	3.89E-07	5.44E-04	0.3053	-1.7118	9.23E-01	9.96E-01	1.0005	0.0006	3.97E-02	9.85E-01	1.7711	0.8246	2.15E-04	7.01E-02	0.5944	-0.7506	3.97E-01	1.00E+00	1.1622	0.2168	7.65E-02	6.33E-01	1.3178	0.3981
DELTA.17-U-46619	Heart	Positive	-	*	-	*	-	-	-	-	3.67E-02	1.64E-01	0.7180	-0.4780	8.13E-01	9.96E-01	0.9465	-0.0794	7.58E-01	9.85E-01	1.1641	0.2192	4.61E-01	9.49E-01	0.9388	-0.0912	9.00E-01	1.00E+00	0.9970	-0.0043	3.02E-01	6.88E-01	1.1133	0.1548
Hypoxanthine	Heart	Positive	*	*	*	*	-	-	-	-	3.27E-01	6.26E-01	1.0834	0.1155	3.81E-01	9.62E-01	0.9336	-0.0992	1.31E-01	9.85E-01	0.8549	-0.2261	1.04E-01	9.40E-01	0.9110	-0.1345	2.33E-01	1.00E+00	1.0888	0.1227	3.10E-01	6.89E-01	1.0675	0.0942
LysoPE(18:0)	Heart	Positive	*	*	*	*	-	-	-	-	1.91E-01	4.83E-01	1.4209	0.5068	6.18E-01	9.96E-01	0.9771	-0.0335	3.32E-01	9.85E-01	0.7852	-0.3488	4.69E-01	9.50E-01	0.9012	-0.1501	5.02E-01	1.00E+00	1.1686	0.2247	1.25E-01	6.47E-01	1.2733	0.3485
Cer(d18:1/20:0)	Heart	Positive	-	-	*	*	-	-	-	-	9.87E-01	9.94E-01	0.9336	-0.0992	2.17E-02	7.87E-01	0.6261	-0.6756	5.63E-01	9.85E-01	0.9299	-0.1049	8.53E-02	9.40E-01	1.9741	0.9812	6.90E-01	1.00E+00	0.8913	-0.1661	2.76E-01	6.80E-01	0.6584	-0.6029
PG(16:0/18:1)	Heart	Positive	*	*	-	*	-	-	-	-	5.54E-01	7.83E-01	1.0782	0.1087	1.29E-02	7.87E-01	0.6449	-0.6329	2.02E-01	9.85E-01	0.8335	-0.2628	1.43E-01	9.40E-01	1.6495	0.7221	8.06E-01	1.00E+00	1.1048	0.1438	4.95E-01	7.27E-01	0.7817	-0.3553
PG(18:1/18:1)	Heart	Positive	*	*	-	*	-	-	-	-	6.54E-01	8.46E-01	1.0541	0.0760	1.06E-01	7.87E-01	0.7883	-0.3432	4.16E-01	9.85E-01	0.8972	-0.1566	1.01E-01	9.40E-01	1.5751	0.6555	9.49E-01	1.00E+00	1.0536	0.0754	5.63E-01	7.62E-01	0.8491	-0.2360
PC(22:6/18:0)	Heart	Positive	*	-	*	*	x	x	-	-	2.57E-03	2.45E-02	1.3541	0.4374	1.38E-01	7.91E-01	0.9273	-0.1089	4.99E-01	9.85E-01	1.0310	0.0440	2.77E-01	9.40E-01	0.9376	-0.0930	5.10E-01	1.00E+00	1.0454	0.0640	1.89E-01	6.56E-01	1.0765	0.1063
Methyl DHA	Heart	Positive	*	-	*	-	-	-	-	-	6.94E-01	8.63E-01	0.9757	-0.0355	5.42E-01	9.96E-01	1.0918	0.1267	3.72E-01	9.85E-01	0.9039	-0.1458	7.53E-01	9.86E-01	0.9776	-0.0327	7.34E-01	1.00E+00	1.0191	0.0273	7.23E-01	8.57E-01	0.9345	-0.0977
LysoPC(16:0)	Heart	Positive	-	-	*	-	-	-	-	-	5.36E-01	7.72E-01	0.8188	-0.2884	5.66E-01	9.96E-01	0.8786	-0.1867	4.49E-01	9.85E-01	0.8215	-0.2837	4.77E-01	9.50E-01	1.0040	0.0057	7.86E-01	1.00E+00	0.9763	-0.0346	1.69E-01	6.56E-01	1.5590	0.6407
Monoolein	Heart	Positive	-	-	*	*	-	-	-	-	8.14E-02	2.82E-01	0.4248	-1.2351	2.65E-01	8.90E-01	0.7076	-0.4991	4.85E-01	9.85E-01	0.8217	-0.2834	1.26E-01	9.40E-01	0.4967	-1.0096	1.17E-01	1.00E+00	1.6979	0.7638	1.16E-01	6.41E-01	2.5384	1.3439
Acetylcarnitine	Heart	Positive	*	*	*	*	-	-	-	-	1.36E-01	3.94E-01	1.3238	0.4046	5.34E-01	9.96E-01	0.8893	-0.1692	2.51E-01	9.85E-01	0.8042	-0.3144	3.51E-02	8.35E-01	0.7238	-0.4663	7.16E-01	1.00E+00	1.1181	0.1610	1.32E-01	6.47E-01	1.3078	0.3871
PG(18:2)	Heart	Positive	*	*	-	*	-	-	-	-	1.32E-01	3.88E-01	1.2203	0.2872	9.88E-02	7.87E-01	0.7996	-0.3227	2.68E-01	9.85E-01	0.8698	-0.2012	5.98E-02	9.40E-01	1.5486	0.6310	8.40E-01	1.00E+00	1.0210	0.0300	7.69E-02	6.33E-01	0.7588	-0.3982
PC(16:0/22:6)	Heart	Positive	*	*	*	*	x	x	-	-	5.41E-03	4.51E-02	1.1827	0.2421	6.09E-02	7.87E-01	0.9090	-0.1376	5.80E-01	9.85E-01	0.9750	-0.0365	1.17E-01	9.40E-01	0.9366	-0.0945	4.47E-01	1.00E+00	1.0404	0.0572	3.84E-01	6.95E-01	1.0330	0.0468
Adrenic Acid (22:4, n-6)	Heart	Positive	*	*	*	*	-	-	-	-	2.32E-02	1.20E-01	0.5632	-0.8283	8.53E-01	9.96E-01	1.0071	0.0102	6.10E-01	9.85E-01	1.2391	0.3093	4.34E-01	9.46E-01	0.9205	-0.1196	8.39E-01	1.00E+00	1.0111	0.0160	2.82E-01	6.80E-01	1.1831	0.2426
Glu	Heart	Positive	*	*	*	-	-	-	-	-	3.39E-01	6.33E-01	1.0395	0.0558	6.34E-01	9.96E-01	0.9837	-0.0237	2.02E-01	9.85E-01	0.9318	-0.1020	9.26E-01	1.00E+00	0.9996	-0.0006	8.67E-01	1.00E+00	1.0098	0.0141	3.32E-01	6.95E-01	0.9517	-0.0715
γ-Homolinolenic acid	Heart	Positive	-	*	*	*	x	x	-	-	3.87E-04	6.27E-03	0.5248	-0.9300	5.62E-01	9.96E-01	0.9460	-0.0801	7.76E-02	9.85E-01	1.5055	0.5902	2.06E-01	9.40E-01	0.8620	-0.2142	8.15E-01	1.00E+00	1.0382	0.0541	8.92E-02	6.38E-01	1.2488	0.3206
DL-Norvaline	Heart	Positive	*	*	*	*	-	-	-	-	2.02E-02	1.10E-01	0.6838	-0.5485	2.46E-01	8.90E-01	1.1285	0.1744	2.43E-02	9.85E-01	1.3294	0.4108	5.63E-03	3.98E-01	0.7143	-0.4853	7.52E-02	1.00E+00	1.2743	0.3497	2.06E-01	6.56E-01	1.1829	0.2424
N-Arachidonoyl-L-serine	Heart	Positive	*	*	-	-	-	-	-	-	9.35E-01	9.74E-01	1.0052	0.0075	3.30E-01	9.14E-01	0.8854	-0.1756	2.17E-01	9.85E-01	0.8268	-0.2745	7.80E-01	9.87E-01	0.9708	-0.0428	4.19E-01	1.00E+00	0.8867	-0.1735	7.22E-01	8.57E-01	0.9433	-0.0842
2-AG	Heart	Positive	*	*	-	*	x	x	-	-	1.85E-03	1.89E-02	0.3498	-1.5154	2.17E-01	8.83E-01	1.6575	0.7290	2.24E-01	9.85E-01	1.5356	0.6188	3.28E-01	9.40E-01	0.8772	-0.1891	9.60E-01	1.00E+00	0.9499	-0.0742	9.58E-02	6.38E-01	1.4437	0.5298
Eicosadienoic acid	Heart	Positive	*	*	-	*	x	x	-	-	2.47E-04	4.61E-03	0.3641	-1.4577	8.09E-01	9.96E-01	1.1897	0.2506	2.86E-01	9.85E-01	1.1410	0.1903	2.24E-01	9.40E-01	0.8135	-0.2978	3.56E-01	1.00E+00	0.8508	-0.2331	1.36E-01	6.51E-01	1.5374	0.6205
LysoPE(16:0)	Heart	Positive	*	*	*	-	x	x	-	-	5.53E-03	4.53E-02	0.4320	-1.2109	1.06E-01	7.87E-01	1.5037	0.5885	6.35E-01	9.85E-01	1.6316	0.7063	1.08E-01	9.40E-01	0.6895	-0.5364	4.46E-01	1.00E+00	1.5574	0.6391	7.00E-01	8.45E-01	0.7681	-0.3807
Gln	Heart	Positive	*	*	-	*	-	-	-	-	2.52E-02	1.27E-01	1.5181	0.6022	2.23E-01	8.83E-01	0.8280	-0.2723	3.50E-02	9.85E-01	0.6852	-0.5455	3.22E-01	9.40E-01	0.8880	-0.1713	4.57E-01	1.00E+00	0.8577	-0.2215	2.67E-01	6.69E-01	1.1960	0.2583
L-Carnitine	Heart	Positive	-	-	*	-	-	-	-	-	1.97E-01	4.89E-01	0.8969	-0.1570	1.33E-01	7.91E-01	0.8805	-0.1836	6.34E-01	9.85E-01	0.9750	-0.0366	3.56E-01	9.40E-01	1.1041	0.1429	1.77E-01	1.00E+00	0.8597	-0.2181	9.63E-01	9.81E-01	1.0176	0.0252
LysoPC(18:0)	Heart	Positive	*	*	-	-	-	-	-	-	2.57E-01	5.56E-01	1.1849	0.2448	6.87E-01	9.96E-01	0.9479	-0.0773	1.60E-01	9.85E-01	0.8006	-0.3208	9.25E-01	1.00E+00	1.0186	0.0265	7.79E-01	1.00E+00	1.0213	0.0304	2.53E-01	6.59E-01	1.1415	0.1909
7α,12α-Dihydroxycholest-4-en-3-one	Heart	Positive	*	*	-	*	x	x	-	-	8.37E-05	2.60E-03	0.2342	-2.0941	2.11E-01	8.79E-01	1.9744	0.9815	9.07E-02	9.85E-01	1.4633	0.5492	3.80E-01	9.40E-01	0.8676	-0.2050	6.97E-01	1.00E+00	0.9870	-0.0189	5.61E-02	6.33E-01	2.2039	1.1401
Arachidonic acid	Heart	Positive	-	-	-	-	-	-	-	-	8.78E-01	9.46E-01	0.9930	-0.0102	6.75E-01	9.96E-01	0.9470	-0.0786	2.49E-01	9.85E-01	0.8434	-0.2458	7.63E-01	9.86E-01	0.9833	-0.0243	3.86E-01	1.00E+00	0.8759	-0.1911	3.34E-01	6.95E-01	0.8661	-0.2074
Creatine	Heart	Positive	*	*	-	*	-	-	-	-	3.24E-01	6.25E-01	1.1094	0.1498	6.53E-02	7.87E-01	0.8132	-0.2983	7.59E-02	9.85E-01	0.8136	-0.2976	5.16E-01	9.55E-01	0.9398	-0.0896	5.77E-01	1.00E+00	0.9126	-0.1319	6.24E-01	7.99E-01	1.0585	0.0821
Methyl ricinoleate	Heart	Positive	*	*	*	-	x	x	-	-	5.91E-04	8.20E-03	0.3962	-1.3357	6.02E-02	7.87E-01	1.5193	0.6034	2.64E-01	9.85E-01	1.2354	0.3050	5.16E-01	9.55E-01	1.1194	0.1628	1.61E-01	1.00E+00	0.7895	-0.3410	3.23E-01	6.95E-01	1.3384	0.4205
Methyl DPA	Heart	Positive	*	*	-	*	x	x	-	-	2.11E-03	2.09E-02	0.3701	-1.4342	3.54E-01	9.39E-01	1.1649	0.2203	7.09E-01	9.85E-01	1.1461	0.1967	6.14E-01	9.70E-01	0.9106	-0.1351	9.00E-01	1.00E+00	0.9867	-0.0194	6.13E-02	6.33E-01	1.5715	0.6522
Erucamide	Heart	Positive	*	*	-	-	-	-	-	-	1.56E-02	9.13E-02	0.6584	-0.6031	5.14E-02	7.87E-01	1.2383	0.3084	7.45E-01	9.85E-01	1.1205	0.1641	7.43E-01	9.85E-01	0.9859	-0.0206	3.88E-01	1.00E+00	0.8824	-0.1805	6.93E-01	8.39E-01	0.9494	-0.0749
9(10)-EpOME	Heart	Positive	*	*	*	*	x	x	-	-	1.70E-03	1.76E-02	0.5273	-0.9233	1.50E-01	8.09E-01	1.1791	0.2377	1.17E-01	9.85E-01	1.3878	0.4728	4.89E-04	9.79E-02	0.6171	-0.6965	1.14E-01	1.00E+00	1.1485	0.1997	2.64E-02	6.33E-01	1.3164	0.3966
N-Arachidonoyl-L-alanine	Heart	Positive	*	*	*	*	x	x	-	-	1.07E-04	3.02E-03	0.2425	-2.0438	1.23E-01	7.91E-01	2.1184	1.0830	8.39E-02	9.85E-01	1.9303	0.9488	3.18E-02	7.96E-01	0.6320	-0.6620	3.34E-01	1.00E+00	1.1267	0.1721	2.20E-02	6.33E-01	1.7613	0.8167
PC(18:0/18:1)	Heart	Positive	*	-	-	*	-	-	-	-	6.53E-01	8.45E-01	1.1733	0.2305	6.54E-01	9.96E-01	0.9936	-0.0093	6.72E-01	9.85E-01	1.0136	0.0195	2.07E-01	9.40E-01	1.2997	0.3782	8.56E-01	1.00E+00	1.0213	0.0304	3.52E-02	6.33E-01	0.6478	-0.6264
2-Linoleoylglycerol	Heart	Positive	*	*	*	*	x	x	-	-	5.98E-05	2.28E-03	0.4460	-1.1650	3.72E-02	7.87E-01	1.4199	0.5058	2.91E-01	9.85E-01	1.3676	0.4516	1.26E-01	9.40E-01	0.7935	-0.3337	2.26E-01	1.00E+00	1.1487	0.2000	9.50E-02	6.38E-01	1.4238	0.5098
15,19-Hhydroxy PGE1	Heart	Positive	-	*	*	-	-	-	-	-	2.46E-01	5.47E-01	0.7283	-0.4574	6.60E-01	9.96E-01	0.9734	-0.0389	9.69E-01	9.93E-01	1.0219	0.0313	6.37E-01	9.70E-01	1.1061	0.1455	5.92E-01	1.00E+00	0.9013	-0.1500	1.59E-01	6.51E-01	1.3873	0.4723
PC(16:0/20:4)	Spleen	Negative	*	-	-	*	x	x	x	-	1.68E-04	1.74E-03	1.2985	0.3769	8.63E-01	9.99E-01	0.9901	-0.0144	6.84E-01	9.07E-01	1.0510	0.0717	1.70E-03	1.08E-02	1.2121	0.2775	5.36E-01	9.99E-01	1.0469	0.0662	4.68E-04	1.39E-02	0.8047	-0.3135
PS(16:0/18:1)	Spleen	Negative	*	*	-	*	x	x	x	-	2.01E-06	4.94E-05	0.6788	-0.5591	3.32E-02	9.73E-01	1.1735	0.2308	4.10E-01	8.36E-01	1.0620	0.0869	1.86E-04	1.83E-03	0.7433	-0.4280	3.60E-03	2.66E-01	0.8104	-0.3034	8.70E-01	9.42E-01	1.0322	0.0457
PC(16:0/18:2)	Spleen	Negative	*	-	-	*	x	x	x	-	3.29E-03	1.85E-02	1.2725	0.3477	8.77E-01	9.99E-01	0.9857	-0.0207	4.37E-01	8.42E-01	1.1434	0.1933	2.52E-03	1.47E-02	1.2789	0.3549	4.09E-01	9.99E-01	1.0952	0.1312	4.38E-03	4.61E-02	0.7792	-0.3600
PS(18:0/20:4)	Spleen	Negative	-	*	*	*	x	x	-	-	5.27E-03	2.63E-02	1.1937	0.2554	1.40E-01	9.73E-01	1.0905	0.1250	1.81E-01	6.66E-01	0.9092	-0.1373	5.36E-02	1.61E-01	1.1608	0.2151	1.15E-01	9.99E-01	0.8770	-0.1893	1.16E-01	3.21E-01	0.8572	-0.2223
PS(18:0/18:1)	Spleen	Negative	-	-	*	*	-	-	-	-	5.51E-01	6.55E-01	1.0434	0.0613	3.90E-02	9.73E-01	1.1632	0.2182	9.12E-01	9.79E-01	1.0180	0.0258	8.18E-02	2.17E-01	1.1578	0.2114	3.66E-01	9.99E-01	0.9212	-0.1184	5.00E-01	7.39E-01	0.9391	-0.0907
PE(16:0/18:2)	Spleen	Negative	*	-	-	-	x	x	-	-	2.01E-05	3.18E-04	0.6136	-0.7047	1.25E-01	9.73E-01	1.1080	0.1480	5.72E-01	8.71E-01	0.9688	-0.0458	4.74E-02	1.47E-01	0.8272	-0.2737	5.89E-02	8.04E-01	0.8417	-0.2486	3.72E-02	1.67E-01	0.8320	-0.2653
Cervonic acid	Spleen	Negative	-	-	-	-	-	-	-	-	8.82E-01	9.16E-01	0.9401	-0.0891	5.20E-01	9.99E-01	0.8615	-0.2151	3.39E-01	8.01E-01	0.8100	-0.3041	1.41E-02	5.69E-02	1.7704	0.8241	3.17E-01	9.99E-01	1.2139	0.2796	5.12E-02	1.97E-01	1.4645	0.5504
PE(18:0/20:4)	Spleen	Negative	*	*	*	*	x	x	-	-	3.71E-03	2.00E-02	0.6432	-0.6366	9.50E-01	9.99E-01	1.0299	0.0425	2.60E-02	4.87E-01	1.2867	0.3637	8.02E-01	8.99E-01	0.9950	-0.0072	7.49E-01	9.99E-01	1.0866	0.1198	1.03E-01	3.01E-01	1.2609	0.3344
ω-3 Arachidonic acid	Spleen	Negative	*	*	-	-	-	-	x	-	2.87E-01	4.28E-01	1.3311	0.4126	9.38E-01	9.99E-01	0.9555	-0.0657	1.62E-01	6.38E-01	0.6655	-0.5876	1.18E-02	4.93E-02	1.8112	0.8569	6.29E-01	9.99E-01	1.0771	0.1072	3.67E-01	6.51E-01	1.2150	0.2810
PS(18:0/18:2)	Spleen	Negative	*	*	-	-	x	x	-	-	2.07E-05	3.26E-04	0.7461	-0.4225	2.36E-02	9.73E-01	1.1644	0.2197	3.69E-01	8.18E-01	1.0690	0.0963	1.13E-01	2.71E-01	0.8777	-0.1882	8.46E-02	9.39E-01	0.8663	-0.2071	8.54E-01	9.32E-01	0.9926	-0.0107
PE(P-18:0/22:6)	Spleen	Negative	-	-	*	-	-	-	x	-	1.84E-01	3.32E-01	0.8307	-0.2676	4.39E-01	9.99E-01	0.9081	-0.1391	1.88E-01	6.74E-01	0.8065	-0.3103	5.76E-03	2.78E-02	1.6116	0.6885	1.33E-01	9.99E-01	0.7652	-0.3861	4.36E-01	7.02E-01	1.1103	0.1510
12(13)-EpOME	Spleen	Negative	*	*	*	*	-	-	-	-	3.59E-01	4.94E-01	0.8709	-0.1995	3.04E-01	9.73E-01	1.0545	0.0766	9.42E-01	9.86E-01	1.7053	0.7701	9.93E-01	9.96E-01	1.2155	0.2815	1.41E-01	9.99E-01	0.5318	-0.9111	7.61E-01	8.83E-01	0.7191	-0.4758
PS(16:0/20:4)	Spleen	Negative	*	-	-	-	x	x	x	-	8.89E-05	1.06E-03	0.7522	-0.4107	9.76E-02	9.73E-01	1.1133	0.1549	7.67E-01	9.32E-01	0.9834	-0.0242	3.92E-05	5.03E-04	0.6725	-0.5723	3.07E-03	2.56E-01	0.7740	-0.3696	3.68E-01	6.51E-01	0.9275	-0.1086
Glu	Spleen	Negative	-	*	*	*	x	x	x	-	8.42E-05	1.02E-03	0.7413	-0.4318	1.84E-02	9.73E-01	0.8527	-0.2300	9.81E-01	9.92E-01	1.0040	0.0058	1.27E-05	2.15E-04	0.6347	-0.6559	3.30E-01	9.99E-01	1.0980	0.1349	4.48E-02	1.83E-01	1.1886	0.2493
PS(18:0/22:6)	Spleen	Negative	-	*	*	*	-	-	-	-	4.12E-01	5.46E-01	1.0810	0.1123	5.19E-01	9.99E-01	1.0510	0.0717	9.43E-01	9.86E-01	0.9934	-0.0095	4.67E-02	1.46E-01	1.1478	0.1988	7.75E-01	9.99E-01	0.9821	-0.0260	2.72E-01	5.54E-01	0.9333	-0.0996
PE(16:0/20:4)	Spleen	Negative	*	-	-	-	x	x	xxx	-	2.70E-05	4.01E-04	0.7299	-0.4542	3.49E-01	9.84E-01	1.0517	0.0727	5.14E-01	8.59E-01	0.9590	-0.0604	2.22E-04	2.12E-03	0.7911	-0.3381	3.60E-05	2.48E-02	0.8041	-0.3145	3.86E-04	1.34E-02	0.8296	-0.2695
Asp	Spleen	Negative	-	*	*	*	-	-	x	-	2.72E-02	8.88E-02	0.8336	-0.2625	4.47E-02	9.73E-01	0.8568	-0.2230	9.50E-01	9.86E-01	1.0029	0.0042	1.38E-05	2.25E-04	0.6026	-0.7308	8.46E-01	9.99E-01	1.0297	0.0422	7.82E-01	8.93E-01	1.0285	0.0406
PE(P-18:0/22:6)	Spleen	Negative	-	*	-	*	x	x	-	-	7.08E-05	9.06E-04	0.4727	-1.0810	6.29E-01	9.99E-01	0.9857	-0.0208	9.71E-01	9.90E-01	1.0814	0.1129	5.99E-02	1.74E-01	0.7237	-0.4666	4.32E-01	9.99E-01	0.8741	-0.1941	2.02E-01	4.57E-01	1.2653	0.3394
Mannose 6-Phosphate	Spleen	Negative	-	*	-	*	-	-	-	-	1.26E-02	5.11E-02	0.7731	-0.3714	8.07E-01	9.99E-01	0.9982	-0.0027	8.93E-01	9.74E-01	1.0063	0.0090	1.67E-02	6.51E-02	0.7825	-0.3539	3.89E-01	9.99E-01	0.8792	-0.1857	3.12E-02	1.53E-01	1.2879	0.3651
GLR	Spleen	Positive	*	*	*	*	x	x	x	-	2.70E-03	1.90E-02	1.3355	0.4174	8.12E-01	9.66E-01	0.9794	-0.0300	7.60E-01	9.25E-01	0.9844	-0.0227	1.68E-03	1.31E-02	1.4569	0.5429	8.03E-01	9.80E-01	0.9837	-0.0237	1.06E-02	1.00E-01	0.7453	-0.4241
PC(16:0/18:1)	Spleen	Positive	-	-	-	-	-	-	-	-	5.09E-01	6.49E-01	0.9726	-0.0400	8.08E-01	9.66E-01	0.9807	-0.0281	2.01E-02	2.07E-01	0.8459	-0.2415	9.64E-02	2.81E-01	0.9523	-0.0706	2.02E-01	7.21E-01	0.9566	-0.0641	6.00E-01	8.02E-01	0.9853	-0.0214
PC(18:0/22:6)	Spleen	Positive	*	-	*	*	-	-	-	-	8.94E-01	9.37E-01	1.0089	0.0128	6.87E-01	9.50E-01	0.9792	-0.0304	4.16E-01	7.97E-01	1.0398	0.0564	2.04E-02	9.73E-02	0.8880	-0.1715	6.10E-02	6.32E-01	1.1078	0.1477	4.02E-03	4.99E-02	1.1828	0.2422
Hypoxanthine	Spleen	Positive	*	*	*	*	x	x	x	-	1.15E-04	1.88E-03	0.5822	-0.7805	7.97E-01	9.65E-01	1.0053	0.0076	6.15E-01	8.86E-01	1.0652	0.0911	6.34E-07	1.62E-05	0.5018	-0.9949	4.41E-01	8.46E-01	1.0889	0.1228	2.93E-04	7.51E-03	1.4745	0.5602
PC(16:1/16:1)	Spleen	Positive	*	-	-	*	x	x	x	-	1.75E-09	6.75E-07	0.6393	-0.6455	6.79E-01	9.42E-01	1.0159	0.0227	7.64E-01	9.25E-01	0.9888	-0.0163	1.12E-08	6.46E-07	0.6209	-0.6877	5.69E-01	9.24E-01	0.9822	-0.0260	5.85E-06	2.55E-04	1.2271	0.2952
LysoPC(17:0)	Spleen	Positive	*	*	*	*	-	-	-	-	4.28E-02	1.29E-01	0.7504	-0.4142	8.95E-01	9.81E-01	1.0275	0.0392	7.20E-01	9.14E-01	1.0938	0.1294	8.25E-01	9.00E-01	0.9947	-0.0077	7.18E-01	9.59E-01	1.0539	0.0757	4.77E-01	7.30E-01	1.0935	0.1290
N-Ac-Phe	Spleen	Positive	*	*	-	-	x	x	-	-	5.69E-03	3.18E-02	1.3291	0.4104	1.78E-01	6.79E-01	0.8673	-0.2055	6.34E-01	8.89E-01	0.9634	-0.0538	4.64E-01	6.77E-01	1.1312	0.1779	7.93E-01	9.76E-01	1.0951	0.1310	1.01E-01	3.50E-01	1.3067	0.3860
LysoPE(16:0)	Spleen	Positive	*	-	*	*	x	x	-	-	6.75E-04	7.46E-03	0.6866	-0.5424	6.10E-01	9.25E-01	1.0326	0.0463	5.71E-01	8.65E-01	0.9637	-0.0533	1.52E-01	3.70E-01	1.1791	0.2377	5.16E-01	8.92E-01	0.9330	-0.1001	4.51E-01	7.16E-01	0.9150	-0.1282
PC(14:0/16:0)	Spleen	Positive	*	-	-	*	x	x	x	-	7.57E-05	1.34E-03	0.6270	-0.6736	7.87E-01	9.65E-01	1.0281	0.0399	3.51E-01	7.50E-01	0.9179	-0.1237	1.06E-04	1.23E-03	0.7469	-0.4210	3.01E-02	6.15E-01	0.8172	-0.2912	3.34E-05	1.21E-03	1.2352	0.3047
11-HEDE	Spleen	Positive	*	*	*	-	-	-	-	-	2.26E-01	3.85E-01	1.3256	0.4066	3.88E-01	8.30E-01	0.8099	-0.3042	1.30E-01	4.90E-01	0.6809	-0.5545	1.01E-02	5.62E-02	1.8189	0.8630	9.99E-01	1.00E+00	0.9581	-0.0617	3.30E-01	6.08E-01	1.2136	0.2793
PC(18:0/18:1)	Spleen	Positive	*	*	*	*	-	-	-	-	1.57E-02	6.43E-02	1.1520	0.2042	4.43E-01	8.60E-01	0.9596	-0.0594	8.97E-02	3.96E-01	0.9074	-0.1402	5.02E-02	1.81E-01	0.9147	-0.1287	3.52E-02	6.15E-01	1.1041	0.1428	2.52E-01	5.25E-01	1.0387	0.0548
L-Valine	Spleen	Positive	-	*	*	*	x	x	x	-	9.29E-07	4.93E-05	0.5822	-0.7805	2.75E-01	7.57E-01	0.9354	-0.0964	3.37E-01	7.39E-01	1.0606	0.0849	1.64E-09	1.21E-07	0.4706	-1.0875	1.04E-01	6.56E-01	1.1617	0.2162	8.88E-09	6.57E-07	1.7597	0.8153
Arachidonic acid	Spleen	Positive	*	*	-	-	-	-	x	-	2.07E-01	3.66E-01	1.4092	0.4949	8.91E-01	9.81E-01	0.9530	-0.0695	2.06E-01	6.28E-01	0.7145	-0.4850	3.81E-03	2.59E-02	1.7899	0.8398	6.91E-01	9.58E-01	1.0544	0.0765	4.65E-01	7.24E-01	1.1283	0.1741
Taurolite	Spleen	Positive	-	-	*	*	x	x	-	-	3.84E-03	2.42E-02	0.6329	-0.6599	4.78E-01	8.78E-01	0.9007	-0.1509	3.30E-01	7.36E-01	0.8693	-0.2021	6.59E-02	2.18E-01	1.3122	0.3919	2.66E-01	7.54E-01	0.8482	-0.2375	7.12E-01	8.69E-01	0.9588	-0.0606
DCHA-PAF	Spleen	Positive	-	*	*	*	x	x	x	-	1.48E-05	3.95E-04	0.7942	-0.3324	6.19E-01	9.27E-01	0.9846	-0.0225	8.87E-01	9.63E-01	1.0081	0.0116	7.03E-09	4.51E-07	0.7149	-0.4842	8.66E-01	9.85E-01	1.0087	0.0126	2.51E-10	4.32E-08	1.7174	0.7802
LysoPC(22:0)	Spleen	Positive	*	*	*	*	-	-	-	-	2.22E-01	3.82E-01	0.9267	-0.1098	5.02E-02	5.44E-01	1.1339	0.1813	5.43E-03	9.66E-02	1.1768	0.2349	4.02E-01	6.28E-01	1.0466	0.0657	4.74E-01	8.67E-01	0.9612	-0.0571	2.20E-01	4.86E-01	0.9228	-0.1160
PC(18:1/14:0)	Spleen	Positive	-	-	-	*	x	x	x	-	2.46E-03	1.81E-02	0.8513	-0.2323	2.03E-01	6.93E-01	0.9391	-0.0906	5.46E-03	9.66E-02	0.8524	-0.2304	5.38E-06	9.40E-05	0.7707	-0.3758	3.90E-03	4.69E-01	0.8651	-0.2090	9.36E-01	9.68E-01	1.0040	0.0058
SM(d18:1/18:1)	Spleen	Positive	-	*	*	*	x	x	x	-	4.78E-05	9.38E-04	1.3619	0.4457	6.56E-01	9.40E-01	1.0302	0.0430	4.10E-02	2.69E-01	0.8382	-0.2546	2.18E-05	3.18E-04	1.3200	0.4005	3.31E-01	8.00E-01	0.9470	-0.0786	5.63E-01	7.77E-01	0.9836	-0.0238
GSSG	Spleen	Positive	*	*	*	*	-	-	x	-	2.38E-02	8.48E-02	0.6096	-0.7140	7.18E-01	9.51E-01	1.0134	0.0193	2.71E-01	6.79E-01	1.3137	0.3936	1.59E-03	1.26E-02	0.4762	-1.0705	9.55E-01	9.99E-01	1.0148	0.0213	4.45E-01	7.09E-01	1.2280	0.2963
SM(d18:1/18:0)	Spleen	Positive	-	*	*	*	-	-	-	-	2.70E-01	4.37E-01	1.1540	0.2066	3.54E-01	8.08E-01	1.0816	0.1132	5.54E-01	8.56E-01	0.9284	-0.1071	3.72E-02	1.48E-01	1.1948	0.2568	4.08E-01	8.31E-01	0.9435	-0.0839	1.16E-03	1.96E-02	0.7137	-0.4866
PC(P-18:0/0:0)	Spleen	Positive	-	*	-	*	x	x	x	-	2.54E-06	1.04E-04	0.3706	-1.4320	5.91E-01	9.19E-01	0.9748	-0.0368	5.19E-01	8.46E-01	1.2651	0.3393	1.33E-04	1.46E-03	0.3465	-1.5293	6.11E-01	9.36E-01	0.8609	-0.2161	4.13E-03	5.03E-02	2.1083	1.0761
Arg	Spleen	Positive	*	*	*	*	x	x	x	-	1.01E-06	5.10E-05	1.8313	0.8729	1.72E-01	6.79E-01	0.8638	-0.2113	2.38E-01	6.64E-01	0.8905	-0.1673	2.29E-05	3.26E-04	1.7485	0.8061	6.58E-01	9.46E-01	0.9633	-0.0539	6.75E-01	8.46E-01	0.9646	-0.0520
3-Indolyllactic acid	Spleen	Positive	-	*	*	*	x	x	x	-	1.44E-05	3.89E-04	0.6111	-0.7104	7.97E-01	9.65E-01	0.9797	-0.0295	9.57E-01	9.85E-01	1.0200	0.0285	1.90E-06	3.88E-05	0.6367	-0.6513	5.74E-01	9.25E-01	1.0919	0.1269	2.71E-03	3.60E-02	1.2511	0.3232
LysoPE(18:0)	Kidney	Negative	*	*	*	*	-	-	-	-	1.03E-01	6.21E-01	0.8810	-0.1828	2.77E-01	4.39E-01	1.0800	0.1110	1.01E-01	3.94E-01	1.1458	0.1964	5.77E-02	2.13E-01	1.2388	0.3090	2.06E-01	7.13E-01	0.8672	-0.2055	1.02E-01	4.70E-01	0.7791	-0.3601
Glu	Kidney	Negative	*	*	*	*	-	-	x	-	4.26E-01	7.74E-01	0.9706	-0.0431	2.74E-01	4.37E-01	1.0557	0.0783	3.20E-02	2.98E-01	1.1654	0.2209	1.03E-06	1.65E-04	0.8040	-0.3148	1.14E-03	1.33E-01	1.1797	0.2384	2.25E-03	7.44E-02	1.2506	0.3226
2-Hydroxypalmitic acid	Kidney	Negative	*	*	-	*	-	-	-	-	2.75E-02	4.02E-01	0.7884	-0.3430	2.23E-01	3.78E-01	1.0561	0.0788	2.23E-03	1.39E-01	1.1811	0.2402	6.25E-01	7.48E-01	1.0588	0.0825	3.08E-01	7.92E-01	1.8416	0.8809	6.24E-01	8.37E-01	0.9436	-0.0838
Citric Acid	Kidney	Negative	*	*	*	*	-	-	-	-	3.49E-01	7.56E-01	0.5742	-0.8004	4.12E-01	5.57E-01	1.1230	0.1673	1.39E-01	4.53E-01	1.2137	0.2794	1.78E-02	1.08E-01	2.6207	1.3899	5.88E-02	5.91E-01	0.4312	-1.2135	2.75E-02	2.76E-01	0.3789	-1.4003
PC(16:0/20:4)	Kidney	Negative	-	*	*	*	-	-	-	-	6.61E-02	5.57E-01	1.1759	0.2337	8.16E-01	8.69E-01	1.0273	0.0388	1.39E-01	4.53E-01	0.8678	-0.2046	4.59E-01	6.25E-01	1.1089	0.1492	4.02E-01	8.09E-01	0.8917	-0.1654	3.13E-01	6.58E-01	0.8724	-0.1970
PC(16:0/18:2)	Kidney	Negative	-	*	*	*	-	-	-	-	1.50E-01	6.79E-01	1.1659	0.2214	9.81E-01	9.87E-01	1.0184	0.0264	2.09E-01	5.24E-01	0.8735	-0.1951	2.94E-01	4.92E-01	0.8687	-0.2031	3.73E-01	8.03E-01	1.1639	0.2190	4.05E-01	7.10E-01	1.2490	0.3207
Cervonic acid	Kidney	Negative	*	*	-	-	-	-	-	-	4.43E-01	7.80E-01	0.9341	-0.0984	2.80E-02	1.36E-01	1.2387	0.3088	1.64E-01	4.77E-01	1.1354	0.1832	1.32E-02	8.73E-02	1.3540	0.4373	2.01E-01	7.12E-01	1.1369	0.1851	3.02E-01	6.50E-01	1.1169	0.1596
PC(16:0/22:6)	Kidney	Negative	*	*	-	-	-	-	-	-	3.90E-01	7.61E-01	1.0549	0.0771	1.34E-01	2.82E-01	0.9132	-0.1310	1.62E-01	4.77E-01	0.8984	-0.1545	4.96E-01	6.56E-01	0.9559	-0.0650	1.00E+00	1.00E+00	0.9860	-0.0203	8.42E-01	9.38E-01	0.9737	-0.0384
PI(18:0/20:4)	Kidney	Negative	-	-	-	*	-	-	-	-	6.87E-01	8.76E-01	1.0845	0.1170	1.93E-01	3.46E-01	1.2592	0.3325	4.71E-01	7.36E-01	1.1715	0.2284	2.11E-01	4.20E-01	0.6943	-0.5263	9.43E-01	9.86E-01	0.8044	-0.3139	3.68E-01	6.97E-01	1.1295	0.1757
PC(18:1/16:0)	Kidney	Negative	*	*	*	*	-	-	-	-	1.75E-01	6.94E-01	1.0717	0.0998	2.69E-02	1.35E-01	0.9101	-0.1359	5.16E-02	3.29E-01	0.9156	-0.1272	8.81E-01	9.25E-01	1.0153	0.0219	7.88E-01	9.47E-01	0.9992	-0.0012	3.96E-01	7.08E-01	0.8757	-0.1915
LysoPE(16:0)	Kidney	Negative	*	*	*	*	-	-	x	-	1.53E-01	6.80E-01	0.9060	-0.1424	9.67E-02	2.38E-01	1.1162	0.1586	7.94E-02	3.64E-01	1.1618	0.2164	3.08E-04	6.50E-03	1.4798	0.5654	1.41E-01	6.65E-01	0.8601	-0.2174	2.56E-02	2.61E-01	0.7454	-0.4239
14(15)-EpEDE	Kidney	Negative	*	*	-	*	-	-	-	-	9.66E-01	9.92E-01	0.9922	-0.0113	8.50E-03	8.91E-02	1.2792	0.3553	2.01E-01	5.18E-01	1.1639	0.2190	6.64E-02	2.28E-01	1.2083	0.2730	7.93E-01	9.48E-01	1.0291	0.0414	6.79E-01	8.64E-01	0.9546	-0.0671

PC(18:0/22:6)	Kidney	Negative	*	*	*	*	-	-	-	-	6.98E-01	8.77E-01	1.0209	0.0298	2.59E-01	4.20E-01	0.8960	-0.1585	4.37E-01	7.15E-01	0.9367	-0.0944	5.10E-01	6.66E-01	0.9287	-0.1068	3.56E-01	8.03E-01	1.2637	0.3377	1.91E-01	5.90E-01	1.3902	0.4753
PS(16:0/20:4)	Kidney	Negative	-	*	*	*	-	-	-	-	2.40E-01	7.35E-01	0.9069	-0.1410	3.91E-01	5.41E-01	0.9195	-0.1211	3.79E-01	6.66E-01	1.0896	0.1238	6.83E-01	7.85E-01	1.0273	0.0388	6.21E-01	8.87E-01	0.9676	-0.0476	4.32E-01	7.28E-01	0.9358	-0.0957
PE(P-18:0/22:6)	Kidney	Negative	-	-	*	*	-	-	x	-	3.91E-01	7.61E-01	1.0761	0.1058	3.59E-01	5.13E-01	1.0879	0.1215	7.41E-01	8.88E-01	1.0355	0.0504	3.66E-03	3.45E-02	1.6061	0.6836	4.33E-02	5.60E-01	0.7634	-0.3894	1.73E-02	2.35E-01	0.6003	-0.7362
PE(18:0/22:6)	Kidney	Negative	-	*	-	*	-	-	-	-	1.77E-01	6.94E-01	0.8958	-0.1587	3.06E-02	1.42E-01	0.8392	-0.2530	9.58E-01	9.80E-01	1.0197	0.0282	6.78E-01	7.82E-01	0.9590	-0.0605	8.34E-01	9.57E-01	0.9845	-0.0225	5.88E-01	8.20E-01	1.0052	0.0075
PC(16:0/18:0)	Kidney	Negative	*	*	-	-	-	-	-	-	7.21E-01	8.83E-01	1.0110	0.0158	1.28E-02	1.01E-01	0.9079	-0.1393	5.14E-02	3.29E-01	0.9043	-0.1451	8.22E-01	8.86E-01	0.9924	-0.0110	8.52E-01	9.61E-01	0.9894	-0.0154	2.26E-01	6.07E-01	0.8767	-0.1899
PG(16:0/18:1)	Kidney	Negative	*	-	*	*	-	-	-	-	7.63E-01	9.06E-01	1.0162	0.0232	3.13E-03	6.06E-02	0.8541	-0.2276	9.35E-01	9.72E-01	1.0034	0.0049	6.72E-02	2.29E-01	0.8977	-0.1557	3.27E-01	8.03E-01	1.0478	0.0674	7.41E-01	8.89E-01	1.0288	0.0409
PS(18:0/22:6)	Kidney	Negative	-	*	-	-	-	-	-	-	3.42E-02	4.40E-01	0.8723	-0.1972	1.79E-03	5.03E-02	0.8045	-0.3139	9.76E-01	9.86E-01	1.0189	0.0270	2.67E-01	4.66E-01	0.9197	-0.1207	2.39E-01	7.44E-01	0.9065	-0.1416	4.26E-01	7.25E-01	0.9313	-0.1026
Phenaceturic acid	Kidney	Negative	-	-	-	-	-	-	-	-	3.56E-02	4.42E-01	1.6147	0.6912	7.93E-01	8.53E-01	1.3144	0.3944	1.39E-01	4.53E-01	1.8027	0.8502	9.40E-03	7.05E-02	4.0261	2.0094	3.08E-01	7.92E-01	1.0913	0.1260	3.61E-01	6.94E-01	1.0333	0.0472
Asp	Kidney	Negative	*	*	*	*	-	-	-	-	9.18E-02	6.03E-01	0.9230	-0.1156	1.42E-02	1.05E-01	1.1405	0.1896	4.41E-02	3.15E-01	1.1469	0.1978	2.19E-02	1.20E-01	0.8859	-0.1748	5.35E-01	8.64E-01	1.0310	0.0440	7.65E-03	1.57E-01	1.1328	0.1799
PS(18:0/20:4)	Kidney	Negative	*	*	*	*	-	-	-	-	1.88E-01	6.97E-01	1.0779	0.1082	4.96E-02	1.74E-01	0.8773	-0.1888	2.71E-01	5.77E-01	0.9278	-0.1081	2.51E-01	4.55E-01	1.1141	0.1559	2.15E-02	4.96E-01	0.7804	-0.3577	6.93E-02	4.11E-01	0.7630	-0.3903
Carbocyclic thromboxane A2	Kidney	Negative	*	*	*	*	-	-	x	-	1.99E-03	1.11E-01	0.5516	-0.8582	1.50E-02	1.06E-01	1.4119	0.4976	3.27E-01	6.29E-01	1.1884	0.2490	1.86E-03	2.16E-02	1.6133	0.6900	5.39E-01	8.64E-01	0.9259	-0.1110	1.48E-03	6.65E-02	0.5963	-0.7460
PS(18:0/0:0)	Kidney	Negative	-	*	*	*	-	-	x	-	3.44E-01	7.51E-01	1.1147	0.1566	1.62E-01	3.15E-01	1.1913	0.2525	6.53E-01	8.41E-01	0.9514	-0.0718	6.99E-07	1.49E-04	3.1595	1.6597	6.09E-02	5.91E-01	0.7247	-0.4645	9.21E-05	1.60E-02	0.4518	-1.1461
LysoPC(18:0)	Kidney	Negative	*	*	*	*	-	-	-	-	2.04E-02	3.46E-01	0.7449	-0.4249	6.58E-02	1.99E-01	1.2387	0.3088	2.55E-03	1.48E-01	1.4852	0.5707	5.29E-01	6.79E-01	0.9554	-0.0658	6.73E-01	9.06E-01	1.0166	0.0238	1.50E-01	5.52E-01	1.2072	0.2716
PC(18:0/18:1)	Kidney	Positive	-	*	*	*	-	-	x	-	1.83E-02	3.40E-01	1.1309	0.1775	2.35E-01	5.86E-01	1.0606	0.0848	4.19E-02	4.73E-01	0.9218	-0.1174	1.09E-03	1.38E-02	1.2546	0.3272	1.86E-02	4.27E-01	0.8746	-0.1933	3.12E-02	4.17E-01	0.7701	-0.3769
Eicosapentaenoic acid	Kidney	Positive	*	*	*	*	-	-	-	-	1.31E-02	2.77E-01	0.6947	-0.5255	1.27E-01	4.78E-01	1.2388	0.3089	5.69E-02	4.73E-01	1.4237	0.5097	5.38E-01	6.86E-01	0.9571	-0.0633	4.19E-02	6.80E-01	1.3265	0.4076	6.80E-01	8.01E-01	1.1376	0.1861
PC(16:1/16:1)	Kidney	Positive	-	*	-	-	-	-	-	-	2.34E-01	5.71E-01	1.0702	0.0979	2.85E-01	6.01E-01	1.0528	0.0742	3.24E-01	5.89E-01	0.9478	-0.0774	1.84E-02	1.20E-01	0.8681	-0.2040	2.02E-01	8.59E-01	0.9401	-0.0891	7.74E-02	4.38E-01	0.8112	-0.3019
Arachidonic acid	Kidney	Positive	*	*	-	*	-	-	-	-	8.18E-01	9.08E-01	0.9934	-0.0096	9.23E-03	1.38E-01	1.2847	0.3614	3.36E-01	5.93E-01	1.1752	0.2329	7.30E-02	2.44E-01	1.2047	0.2687	6.23E-01	9.13E-01	1.0591	0.0829	1.35E-01	4.42E-01	0.8210	-0.2846
PC(P-18:0/20:4)	Kidney	Positive	-	-	*	*	-	-	x	-	6.75E-01	8.35E-01	0.9616	-0.0565	1.87E-01	5.64E-01	0.9041	-0.1454	7.83E-01	8.77E-01	0.9769	-0.0338	2.01E-06	1.86E-04	0.6298	-0.6670	7.02E-04	5.72E-02	1.3719	0.4561	1.04E-01	4.38E-01	1.5037	0.5885
PC(18:1/14:0)	Kidney	Positive	*	*	*	*	-	-	-	-	8.55E-01	9.25E-01	1.0092	0.0132	4.50E-01	7.23E-01	0.9421	-0.0860	1.25E-01	4.82E-01	0.8834	-0.1789	4.87E-01	6.41E-01	1.0481	0.0678	1.80E-02	4.23E-01	0.8516	-0.2318	2.25E-02	3.77E-01	0.7099	-0.4944
Arachidonoyl Thio-PC	Kidney	Positive	-	*	*	*	-	-	-	-	1.22E-01	5.52E-01	1.0747	0.1039	4.72E-02	2.93E-01	1.0826	0.1145	1.04E-01	4.73E-01	0.9363	-0.0950	1.14E-02	8.70E-02	1.1696	0.2260	1.25E-01	8.59E-01	0.9239	-0.1142	9.31E-02	4.38E-01	0.8025	-0.3174
PC(O-16:0/22:6)	Kidney	Positive	-	*	*	*	-	-	x	-	8.45E-01	9.19E-01	0.9821	-0.0261	1.90E-01	5.64E-01	0.9125	-0.1321	8.88E-01	9.32E-01	1.0091	0.0131	2.24E-06	1.86E-04	0.6417	-0.6401	2.28E-04	5.72E-02	1.3956	0.4809	7.14E-02	4.38E-01	1.5572	0.6390
LysoPC(O-18:0)	Kidney	Positive	*	*	*	*	-	-	-	-	1.02E-01	5.52E-01	0.6853	-0.5451	1.37E-02	1.56E-01	1.3270	0.4082	8.60E-02	4.73E-01	1.3757	0.4602	1.81E-02	1.19E-01	1.4744	0.5601	5.57E-01	8.91E-01	0.9069	-0.1410	1.23E-01	4.38E-01	0.7375	-0.4393
PC(16:0/20:5)	Kidney	Positive	*	*	*	*	-	-	-	-	8.39E-02	5.52E-01	0.8902	-0.1678	3.02E-02	2.29E-01	1.1078	0.1477	1.69E-01	5.07E-01	1.1016	0.1396	7.37E-01	8.33E-01	1.0246	0.0350	9.50E-01	9.90E-01	0.9967	-0.0048	2.57E-01	5.35E-01	0.9145	-0.1290
Phe	Kidney	Positive	*	*	-	-	-	-	-	-	9.42E-01	9.77E-01	0.9680	-0.0469	7.17E-04	7.34E-02	1.6874	0.7548	1.04E-01	4.73E-01	1.5374	0.6205	2.38E-01	4.21E-01	1.2103	0.2754	1.80E-01	8.59E-01	1.2941	0.3720	3.07E-01	5.64E-01	1.4774	0.5631
Sphingomyelin	Kidney	Positive	*	*	-	-	-	-	-	-	7.91E-01	8.93E-01	1.0124	0.0177	4.43E-01	7.23E-01	0.9485	-0.0762	2.73E-01	5.54E-01	0.9385	-0.0916	7.71E-01	8.49E-01	0.9747	-0.0370	3.81E-02	6.39E-01	0.8644	-0.2102	4.94E-02	4.31E-01	0.7382	-0.4380
Hypoxanthine	Kidney	Positive	-	-	*	*	-	-	-	-	5.04E-01	7.35E-01	1.0374	0.0530	7.87E-04	7.34E-02	1.1750	0.2327	1.91E-01	5.14E-01	1.1339	0.1813	8.04E-01	8.70E-01	0.9901	-0.0144	1.54E-01	8.59E-01	1.0849	0.1176	7.01E-01	8.06E-01	1.0497	0.0700
Niacinamide	Kidney	Positive	*	*	-	*	-	-	-	-	8.01E-01	8.96E-01	0.9641	-0.0527	3.25E-03	9.92E-02	1.1722	0.2292	1.75E-01	5.08E-01	1.1544	0.2071	8.26E-01	8.82E-01	1.0109	0.0156	6.94E-01	9.23E-01	1.0359	0.0508	5.45E-01	7.04E-01	0.9632	-0.0541
LysoPC(16:0)	Kidney	Positive	*	*	*	*	-	-	x	-	8.28E-01	9.12E-01	0.9472	-0.0783	4.51E-03	1.05E-01	1.2126	0.2781	5.65E-01	7.56E-01	1.1025	0.1407	1.96E-03	1.99E-02	1.2897	0.3671	6.58E-01	9.13E-01	0.9684	-0.0463	9.39E-02	4.38E-01	0.8030	-0.3165

Table 6A. Pathways Analysis of Amifostine Protection
Amifostine 50 mg

Heart	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Limonene and pinene degradation	5(10)	3.36E-04	-	-
Pentose and Glucuronate Interconversions	-	-	1(1)	1.85E-03
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	2(3)	7.90E-03	-	-
Selenoamino acid metabolism	-	-	1(4)	1.07E-02
Vitamin B3 (nicotinate and nicotinamide) metabolism	-	-	1(4)	1.07E-02
Pentose phosphate pathway	-	-	1(5)	1.46E-02
Saturated fatty acids beta-oxidation	-	-	1(5)	1.46E-02
Xenobiotics metabolism	-	-	1(5)	1.46E-02
Phosphatidylinositol phosphate metabolism	-	-	1(8)	2.41E-02
Fatty Acid Metabolism	-	-	1(8)	2.41E-02
Pyrimidine metabolism	-	-	1(9)	2.69E-02
Purine metabolism	-	-	1(9)	2.69E-02
Glycerophospholipid metabolism	6(33)	2.97E-02	-	-
Fructose and mannose metabolism	1(1)	3.26E-02	-	-
Nucleotide Sugar Metabolism	1(1)	3.26E-02	-	-
Fatty acid activation	-	-	1(15)	3.87E-02
Glycosphingolipid metabolism	-	-	1(16)	4.07E-02
De novo fatty acid biosynthesis	-	-	1(23)	4.82E-02
Sialic acid metabolism	2(7)	4.96E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Table 6B. Pathways Analysis of Amifostine Protection
Amifostine 50 mg

Spleen	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Aspartate and asparagine metabolism	7(13)	8.40E-05	2(7)	2.97E-02
Valine, leucine and isoleucine degradation	4(7)	4.20E-04	2(7)	4.20E-02
Glycosphingolipid metabolism	-	-	3(6)	1.51E-03
Histidine metabolism	3(5)	2.02E-03	-	-
Pyrimidine metabolism	5(16)	2.02E-03	-	-
Nitrogen metabolism	2(2)	4.03E-03	-	-
Beta-Alanine metabolism	3(6)	4.37E-03	-	-
Glutathione Metabolism	3(6)	4.37E-03	-	-
Vitamin B3 (nicotinate and nicotinamide) metabolism	3(6)	4.37E-03	-	-
Squalene and cholesterol biosynthesis	-	-	2(2)	4.54E-03
Methionine and cysteine metabolism	4(12)	5.46E-03	-	-
Purine metabolism	4(13)	6.30E-03	-	-
Glutamate metabolism	3(7)	6.72E-03	2(7)	4.20E-02
Alanine and Aspartate Metabolism	3(7)	6.72E-03	-	-
Butanoate metabolism	3(7)	6.72E-03	3(7)	7.39E-03
Glycine, serine, alanine and threonine metabolism	4(14)	8.82E-03	-	-
Arginine and Proline Metabolism	3(8)	9.24E-03	-	-
Tryptophan metabolism	3(9)	1.32E-02	-	-
Putative anti-Inflammatory metabolites formation from EPA	2(4)	1.49E-02	-	-
Urea cycle/amino group metabolism	3(10)	1.61E-02	-	-
Lysine metabolism	2(5)	2.23E-02	-	-
Bile acid biosynthesis	3(12)	2.39E-02	-	-
Leukotriene metabolism	3(12)	2.39E-02	-	-
Aminosugars metabolism	2(6)	3.28E-02	-	-
Lipoate metabolism	-	-	1(1)	3.48E-02
N-Glycan Degradation	-	-	1(1)	3.48E-02
C21-steroid hormone biosynthesis and metabolism	2(7)	3.67E-02	-	-
Vitamin B2 (riboflavin) metabolism	1(1)	3.68E-02	-	-
Alkaloid biosynthesis II	1(1)	3.68E-02	-	-
Vitamin B1 (thiamin) metabolism	1(1)	3.68E-02	-	-
Vitamin E metabolism	1(1)	3.68E-02	-	-
Mono-unsaturated fatty acid beta-oxidation	1(1)	3.68E-02	-	-
Ubiquinone Biosynthesis	1(1)	3.68E-02	-	-
Arachidonic acid metabolism	3(14)	3.73E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Table 6C. Pathways Analysis of Amifostine Protection
Amifostine 50 mg

Kidney	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Beta-Alanine metabolism	-	-	5(6)	6.72E-04
Glutathione Metabolism	-	-	3(3)	3.87E-03
Vitamin A (retinol) metabolism	5(7)	4.61E-02	3(9)	6.97E-03
Glycerophospholipid metabolism	11(19)	2.97E-02	3(10)	9.16E-03
Glycine, serine, alanine and threonine metabolism	-	-	6(13)	1.14E-02
Vitamin D3 (cholecalciferol) metabolism	4(4)	1.21E-02	-	-
Histidine metabolism	-	-	3(4)	1.31E-02
Tryptophan metabolism	3(4)	1.49E-02	-	-
Tyrosine metabolism	6(11)	1.58E-02	-	-
Vitamin B9 (folate) metabolism	-	-	1(1)	1.86E-02
Linoleate metabolism	6(8)	1.98E-02	-	-
Methionine and cysteine metabolism	-	-	5(11)	2.10E-02
Glutamate metabolism	-	-	3(5)	2.76E-02
Omega-3 fatty acid metabolism	3(3)	3.15E-02	-	-
Sialic acid metabolism	-	-	1(2)	4.22E-02
Hexose phosphorylation	-	-	1(2)	4.22E-02
Ubiquinone Biosynthesis	-	-	1(2)	4.22E-02
Purine metabolism	3(5)	4.67E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Table 6D. Pathways Analysis of Amifostine Protection
Amifostine 200 mg

Heart	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Fatty acid activation	-	-	6(15)	1.68E-04
De novo fatty acid biosynthesis	-	-	7(23)	6.72E-04
Xenobiotics metabolism	-	-	3(5)	2.27E-03
Fructose and mannose metabolism	1(1)	5.80E-03	-	-
Nucleotide Sugar Metabolism	1(1)	5.80E-03	-	-
Linoleate metabolism	-	-	4(12)	5.88E-03
Fatty Acid Metabolism	-	-	3(8)	8.65E-03
Polyunsaturated fatty acid biosynthesis	1(2)	1.13E-02	-	-
Glycolysis and Gluconeogenesis	1(2)	1.13E-02	-	-
Hexose phosphorylation	1(2)	1.13E-02	-	-
Galactose metabolism	1(2)	1.13E-02	-	-
Arachidonic acid metabolism	-	-	3(9)	1.21E-02
Omega-3 fatty acid metabolism	-	-	2(4)	1.27E-02
Pyrimidine metabolism	2(9)	1.37E-02	-	-
Glycosphingolipid metabolism	-	-	4(16)	1.51E-02
Starch and Sucrose Metabolism	1(3)	2.03E-02	-	-
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	1(3)	2.03E-02	-	-
Saturated fatty acids beta-oxidation	-	-	2(5)	2.12E-02
N-Glycan biosynthesis	1(4)	2.64E-02	-	-
Nitrogen metabolism	1(2)	2.66E-02	-	-
Valine, leucine and isoleucine degradation	1(2)	2.66E-02	-	-
Fatty acid oxidation, peroxisome	-	-	1(1)	2.92E-02
Aminosugars metabolism	1(5)	3.51E-02	-	-
Pentose phosphate pathway	1(5)	3.51E-02	-	-
Arginine and Proline Metabolism	1(3)	4.18E-02	-	-
Butanoate metabolism	1(3)	4.18E-02	-	-
Alanine and Aspartate Metabolism	1(3)	4.18E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Table 6E. Pathways Analysis of Amifostine Protection
Amifostine 200 mg

Spleen	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Glycolysis and Gluconeogenesis	-	-	7(7)	5.88E-04
Pentose phosphate pathway	-	-	7(9)	6.72E-04
Glycine, serine, alanine and threonine metabolism	-	-	8(10)	7.56E-04
Tryptophan metabolism	4(9)	1.26E-03	7(9)	8.82E-03
Aspartate and asparagine metabolism	3(13)	3.25E-02	6(7)	1.43E-03
Fructose and mannose metabolism	-	-	5(6)	3.53E-03
Prostaglandin formation from arachidonate	6(11)	4.45E-03	-	-
Vitamin B3 (nicotinate and nicotinamide) metabolism	3(6)	4.71E-03	5(6)	1.56E-02
Pyruvate Metabolism	-	-	5(5)	4.96E-03
Butanoate metabolism	1(2)	1.97E-02	6(7)	6.81E-03
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	6(7)	6.81E-03
Galactose metabolism	-	-	6(7)	6.81E-03
Polyunsaturated fatty acid biosynthesis	1(1)	7.73E-03	-	-
Valine, leucine and isoleucine degradation	1(3)	2.77E-02	3(3)	8.57E-03
Pyrimidine metabolism	4(16)	1.43E-02	3(3)	8.57E-03
Lysine metabolism	-	-	3(3)	8.57E-03
Purine metabolism	-	-	4(5)	1.03E-02
Fatty acid activation	4(7)	1.08E-02	-	-
TCA cycle	-	-	4(4)	1.21E-02
Propanoate metabolism	-	-	4(4)	1.21E-02
Glycerophospholipid metabolism	-	-	9(19)	1.32E-02
Urea cycle/amino group metabolism	3(10)	1.77E-02	-	-
Fatty Acid Metabolism	3(5)	1.88E-02	-	-
De novo fatty acid biosynthesis	5(12)	2.56E-02	-	-
Drug metabolism - cytochrome P450	-	-	3(4)	2.92E-02
Glutamate metabolism	2(7)	4.89E-02	3(4)	3.03E-02
Glutathione Metabolism	-	-	3(4)	3.03E-02
Putative anti-Inflammatory metabolites formation from EPA	-	-	2(2)	3.18E-02
Histidine metabolism	-	-	2(2)	3.18E-02
Arginine and Proline Metabolism	-	-	2(2)	3.18E-02
Beta-Alanine metabolism	2(6)	3.53E-02	2(2)	3.18E-02
Trihydroxycoprostanoyl-CoA beta-oxidation	-	-	2(2)	3.18E-02
Glycosphingolipid metabolism	3(6)	3.39E-02	-	-
Aminosugars metabolism	2(6)	3.53E-02	-	-
Fatty acid oxidation, peroxisome	-	-	2(2)	3.74E-02
Parathio degradation	1(1)	3.92E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Table 6F. Pathways Analysis of Amifostine Protection
Amifostine 200 mg

Kidney	SD 4		SD 9	
Pathway	***overlap size***	***p-value***	***overlap size***	***p-value***
Beta-Alanine metabolism	6(6)	1.09E-03	6(6)	5.88E-04
Valine, leucine and isoleucine degradation	2(3)	7.56E-04	-	-
Butanoate metabolism	8(10)	1.51E-03	-	-
Tryptophan metabolism	2(4)	1.76E-03	3(10)	2.34E-02
Pyruvate Metabolism	5(5)	2.27E-03	-	-
Aspartate and asparagine metabolism	10(15)	2.69E-03	-	-
Ascorbate (Vitamin C) and Aldarate Metabolism	4(8)	2.86E-03	6(8)	7.31E-03
Alanine and Aspartate Metabolism	6(7)	3.19E-03	-	-
Methionine and cysteine metabolism	8(11)	3.36E-03	1(3)	2.20E-02
Vitamin B9 (folate) metabolism	-	-	1(1)	5.55E-03
Histidine metabolism	4(4)	5.97E-03	3(4)	4.68E-02
Vitamin B3 (nicotinate and nicotinamide) metabolism	-	-	3(6)	7.31E-03
Glycerophospholipid metabolism	4(19)	3.65E-02	2(10)	7.65E-03
Pentose phosphate pathway	3(7)	1.14E-02	-	-
Sialic acid metabolism	3(8)	1.60E-02	1(2)	1.34E-02
Chondroitin sulfate degradation	2(3)	1.47E-02	-	-
Glycosphingolipid biosynthesis - globoseries	2(3)	1.47E-02	-	-
Glyoxylate and Dicarboxylate Metabolism	2(3)	1.47E-02	-	-
Glycine, serine, alanine and threonine metabolism	8(13)	1.54E-02	1(5)	3.62E-02
Biopterin metabolism	-	-	2(4)	1.87E-02
Arginine and Proline Metabolism	6(9)	2.03E-02	-	-
Aminosugars metabolism	6(9)	2.03E-02	-	-
Phosphatidylinositol phosphate metabolism	3(9)	2.06E-02	-	-
Glutathione Metabolism	3(3)	2.08E-02	-	-
Vitamin B1 (thiamin) metabolism	3(3)	2.08E-02	-	-
Glycosphingolipid metabolism	-	-	1(3)	2.20E-02
Selenoamino acid metabolism	-	-	1(3)	2.20E-02
Heparan sulfate degradation	2(4)	2.24E-02	-	-
Glycosphingolipid biosynthesis - ganglioseries	2(4)	2.24E-02	-	-
Glycolysis and Gluconeogenesis	5(7)	2.25E-02	-	-
Glutamate metabolism	4(5)	2.39E-02	-	-
Purine metabolism	8(14)	2.49E-02	-	-
Vitamin B6 (pyridoxine) metabolism	1(2)	2.55E-02	-	-
Propanoate metabolism	1(2)	2.57E-02	-	-
Leukotriene metabolism	-	-	1(4)	2.98E-02
Pentose and Glucuronate Interconversions	2(5)	3.34E-02	-	-
Urea cycle/amino group metabolism	-	-	3(12)	3.74E-02
Parathio degradation	-	-	1(1)	4.13E-02
Ubiquinone Biosynthesis	-	-	1(2)	4.57E-02
Hexose phosphorylation	-	-	1(2)	4.57E-02
N-Glycan biosynthesis	2(6)	4.77E-02	-	-
N-Glycan Degradation	1(1)	4.81E-02	-	-
Proteoglycan biosynthesis	1(1)	4.81E-02	-	-
Keratan sulfate degradation	1(1)	4.81E-02	-	-

Note. Pathway analysis result with positive mode and negative mode combined.

[a] Numbers in parenthesis indicates the pathway size.

Heart

SD 4

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
Limonene and pinene degradation	5	10	3.36E-04	E474,E14,E169,E347,E402	C06306,C02759/C11409/C02452/C00964,C02759/C11409/C02452/C00964,C06099/C06078/C00521,C02576	S(+)-trans-Carveol; (4S,6R)-trans-Carveol/Perillyl alcohol; (-)-Perillyl alcohol; p-Mentha-1,8-dien-7-ol; (-)-Perillylalcohol/(-)-trans-Carveol$(+)-trans-Carveol; (4S,6R)-trans-Carveol/Perillyl alcohol; (-)-Perillyl alcohol; p-Mentha-1,8-dien-7-ol; (-)-Perillylalcohol/(-)-trans-Carveol$(+)-Limonene; (+)-(R)-Limonene; (+)-(
Pentose and Glucuronate Interconversions	-	-	-	-	-	-
Carbon fixation	-	-	-	-	-	-
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	2	3	0.007898496	E912,E222	C00165,C00092/C02965/C05345/C00085/C00103/C02976/C01171/C01177/C03735/C00636/C01172/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	Diacylglycerol; Diglyceride$D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate,
Selenoamino acid metabolism	-	-	-	-	-	-
Vitamin B3 (nicotinate and nicotinamide) metabolism	-	-	-	-	-	-
Pentose phosphate pathway	-	-	-	-	-	-
Saturated fatty acids beta-oxidation	-	-	-	-	-	-
Xenobiotics metabolism	-	-	-	-	-	-
Phosphatidylinositol phosphate metabolism	-	-	-	-	-	-
Fatty Acid Metabolism	-	-	-	-	-	-
Pyrimidine metabolism	-	-	-	-	-	-
Purine metabolism	-	-	-	-	-	-
Glycerophospholipid metabolism	6	33	0.029661373	E730,E912,E763,E143,E222,E150	C00319/C02934,C00165,C01595,C00219,C00092/C02965/C05345/C00085/C00103/C02976/C01171/C01177/C03735/C00636/C01172/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075,C00307	Sphingosine; Sphingenine; Sphingoid; Sphing-4-enine/3-Dehydrosphinganine; 3-Dehydro-D-sphinganine$Diacylglycerol; Diglyceride$Linoleate; Linoleic acid; (9Z,12Z)-Octadecadienoic acid; 9-cis,12-cis-Octadecadienoate; 9-cis,12-cis-Octadecadienoic acid$(5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arach
Fructose and mannose metabolism	1	1	0.032602302	E222	C00092/C02965/C05345/C00085/C00103/C02976/C01171/C01177/C03735/C00636/C01172/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Nucleotide Sugar Metabolism	1	1	0.032602302	E222	C00092/C02965/C05345/C00085/C00103/C02976/C01171/C01177/C03735/C00636/C01172/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Fatty acid activation	-	-	-	-	-	-
Glycosphingolipid metabolism	-	-	-	-	-	-
De novo fatty acid biosynthesis	-	-	-	-	-	-
Sialic acid metabolism	2	7	0.049575666	E912,E222	C00165,C00092/C02965/C05345/C00085/C00103/C02976/C01171/C01177/C03735/C00636/C01172/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	Diacylglycerol; Diglyceride$D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate,

Spleen

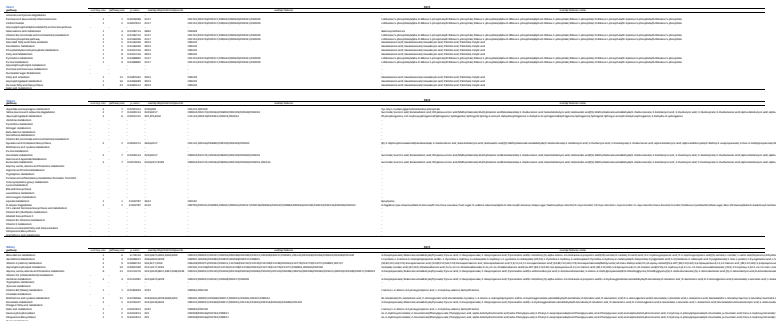
SD 4

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
Aspartate and asparagine metabolism	7	13	8.40E-05	E701,E540,E719,E358,E69,E351,E514	C00217/C05938/C00025,C02238,C00402/C00049,C00362/C00020,C01026/C01205/C02356/C00334/C03284/C05145,C04281/C04282/C01879,C00051	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$5-Oxo-L-proline$D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$dGMP; 2'-Deoxyguanosine 5'-monophos
Valine, leucine and isoleucine degradation	4	7	4.20E-04	E69,E701,E358,E120	C01026/C01205/C02356/C00334/C03284/C05145,C00217/C05938/C00025,C00362/C00020,C00407/C00123	N,N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-methylpropanoate; D-3-Amino-isobutanoate/(S)-2-Aminobutanoate; (S)-2-Aminobutanoic acid; (S)-2-Aminobutyric acid/4-Aminobutanoate; 4-Aminobutanoic acid; 4-Aminobutyrate; 4-Aminobutyric acid; gamma-Aminobutyric acid/L-3-Amino-isobutanoate
Glycosphingolipid metabolism	-	-	-	-	-	-
Histidine metabolism	3	5	0.002016637	E514,E701,E358	C00051,C00217/C05938/C00025,C00362/C00020	Glutathione; 5-L-Glutamyl-L-cysteinylglycine; N-(N-gamma-L-Glutamyl-L-cysteinyl)glycine; gamma-L-Glutamyl-L-cysteinyl-glycine; GSH; Reduced glutathione$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutamin
Pyrimidine metabolism	5	16	0.002016637	E719,E701,E69,E358,E49	C00402/C00049,C00217/C05938/C00025,C01026/C01205/C02356/C00334/C03284/C05145,C00362/C00020,C00055	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$N,N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-met
Nitrogen metabolism	2	2	0.004033275	E719,E701	C00402/C00049,C00217/C05938/C00025	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate
Beta-Alanine metabolism	3	6	0.004369381	E719,E701,E69	C00402/C00049,C00217/C05938/C00025,C01026/C01205/C02356/C00334/C03284/C05145	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$N,N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-met
Glutathione Metabolism	3	6	0.004369381	E514,E701,E351	C00051,C00217/C05938/C00025,C04281/C04282/C01879	Glutathione; 5-L-Glutamyl-L-cysteinylglycine; N-(N-gamma-L-Glutamyl-L-cysteinyl)glycine; gamma-L-Glutamyl-L-cysteinyl-glycine; GSH; Reduced glutathione$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutamin
Vitamin B3 (nicotinate and nicotinamide) metabolism	3	6	0.004369381	E719,E701,E358	C00402/C00049,C00217/C05938/C00025,C00362/C00020	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyg
Squalene and cholesterol biosynthesis	-	-	-	-	-	-
Methionine and cysteine metabolism	4	12	0.005461726	E514,E701,E358,E657	C00051,C00217/C05938/C00025,C00362/C00020,C00302	Glutathione; 5-L-Glutamyl-L-cysteinylglycine; N-(N-gamma-L-Glutamyl-L-cysteinyl)glycine; gamma-L-Glutamyl-L-cysteinyl-glycine; GSH; Reduced glutathione$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutamin
Purine metabolism	4	13	0.006301991	E719,E701,E358,E113	C00402/C00049,C00217/C05938/C00025,C00362/C00020,C00366	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyg
Glutamate metabolism	3	7	0.006722124	E69,E701,E514	C01026/C01205/C02356/C00334/C03284/C05145,C00217/C05938/C00025,C00051	N,N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-methylpropanoate; D-3-Amino-isobutanoate/(S)-2-Aminobutanoate; (S)-2-Aminobutanoic acid; (S)-2-Aminobutyric acid/4-Aminobutanoate; 4-Aminobutanoic acid; 4-Aminobutyrate; 4-Aminobutyric acid; gamma-Aminobutyric acid/L-3-Amino-isobutanoate
Alanine and Aspartate Metabolism	3	7	0.006722124	E719,E701,E358	C00402/C00049,C00217/C05938/C00025,C00362/C00020	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyg
Butanoate metabolism	3	7	0.006722124	E69,E701,E358	C01026/C01205/C02356/C00334/C03284/C05145,C00217/C05938/C00025,C00362/C00020	N,N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-methylpropanoate; D-3-Amino-isobutanoate/(S)-2-Aminobutanoate; (S)-2-Aminobutanoic acid; (S)-2-Aminobutyric acid/4-Aminobutanoate; 4-Aminobutanoic acid; 4-Aminobutyrate; 4-Aminobutyric acid; gamma-Aminobutyric acid/L-3-Amino-isobutanoate
Glycine, serine, alanine and threonine metabolism	4	14	0.008822788	E69,E701,E358,E514	C01026/C01205/C02356/C00334/C03284/C05145,C00217/C05938/C00025,C00362/C00020,C00051	N,N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-methylpropanoate; D-3-Amino-isobutanoate/(S)-2-Aminobutanoate; (S)-2-Aminobutanoic acid; (S)-2-Aminobutyric acid/4-Aminobutanoate; 4-Aminobutanoic acid; 4-Aminobutyrate; 4-Aminobutyric acid; gamma-Aminobutyric acid/L-3-Amino-isobutanoate
Arginine and Proline Metabolism	3	8	0.009242921	E719,E701,E351	C00402/C00049,C00217/C05938/C00025,C04281/C04282/C01879	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$L-1-Pyrroline-3-hydroxy-5-carboxylate; 3-Hydroxy-L-1-pyr
Tryptophan metabolism	3	9	0.013192169	E514,E701,E358	C00051,C00217/C05938/C00025,C00362/C00020	Glutathione; 5-L-Glutamyl-L-cysteinylglycine; N-(N-gamma-L-Glutamyl-L-cysteinyl)glycine; gamma-L-Glutamyl-L-cysteinyl-glycine; GSH; Reduced glutathione$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutamin
Putative anti-Inflammatory metabolites formation from EPA	2	4	0.0148727	E514,E701	C00051,C00217/C05938/C00025	Glutathione; 5-L-Glutamyl-L-cysteinylglycine; N-(N-gamma-L-Glutamyl-L-cysteinyl)glycine; gamma-L-Glutamyl-L-cysteinyl-glycine; GSH; Reduced glutathione$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutamin
Urea cycle/amino group metabolism	3	10	0.016133098	E719,E701,E69	C00402/C00049,C00217/C05938/C00025,C01026/C01205/C02356/C00334/C03284/C05145	D-Aspartate; D-Aspartic acid/L-Aspartate; L-Aspartic acid; 2-Aminosuccinic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$N,N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-met
Lysine metabolism	2	5	0.022267036	E701,E358	C00217/C05938/C00025,C00362/C00020	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/A
Bile acid biosynthesis	3	12	0.023947567	E424,E358,E581	C04483/C02528,C00362/C00020,C15517	3alpha,12alpha-Dihydroxy-5beta-cholanate; Deoxycholic acid; Deoxycholate; 3alpha,12alpha-Dihydroxy-5beta-cholanic acid/Chenodeoxycholate; Chenodeoxycholic acid; 3alpha,7alpha-Dihydroxy-5beta-cholanic acid; Chenodiol$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; De
Leukotriene metabolism	3	12	0.023947567	E514,E358,E657	C00051,C00362/C00020,C00302	Glutathione; 5-L-Glutamyl-L-cysteinylglycine; N-(N-gamma-L-Glutamyl-L-cysteinyl)glycine; gamma-L-Glutamyl-L-cysteinyl-glycine; GSH; Reduced glutathione$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine
Aminosugars metabolism	2	6	0.032770355	E701,E49	C00217/C05938/C00025,C00055	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$CMP; Cytidine-5'-monophosphate; Cytidylic acid
Lipoate metabolism	-	-	-	-	-	-
N-Glycan Degradation	-	-	-	-	-	-
C21-steroid hormone biosynthesis and metabolism	2	7	0.036719603	E484,E407	C05487/C05475/C05478,C05472	17alpha,21-Dihydroxypregnenolone/11beta,21-Dihydroxy-5beta-pregnane-3,20-dione; 5beta-Pregnane-11beta,21-diol-3,20-dione/3alpha,21-Dihydroxy-5beta-pregnane-11,20-dione; 5beta-Pregnane-3alpha,21-diol-11,20-dione$Urocortisol; 5beta-Pregnane-3alpha,11beta,17alpha,21-tetrol-20-one
Vitamin B2 (riboflavin) metabolism	1	1	0.03680363	E358	C00362/C00020	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate
Alkaloid biosynthesis II	1	1	0.03680363	E358	C00362/C00020	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate
Vitamin B1 (thiamin) metabolism	1	1	0.03680363	E358	C00362/C00020	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate
Vitamin E metabolism	1	1	0.03680363	E358	C00362/C00020	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate
Mono-unsaturated fatty acid beta-oxidation	1	1	0.03680363	E358	C00362/C00020	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate
Ubiquinone Biosynthesis	1	1	0.03680363	E358	C00362/C00020	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate
Arachidonic acid metabolism	3	14	0.037307789	E514,E701,E358	C00051,C00217/C05938/C00025,C00362/C00020	Glutathione; 5-L-Glutamyl-L-cysteinylglycine; N-(N-gamma-L-Glutamyl-L-cysteinyl)glycine; gamma-L-Glutamyl-L-cysteinyl-glycine; GSH; Reduced glutathione$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutamin

Kidney

SD 4

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds	overlap features	overlap features name
Beta-Alanine metabolism	-	-	-	-	-	-
Glutathione Metabolism	-	-	-	-	-	-
Vitamin A (retinol) metabolism	5	7	0.046130577	E761,E228,E432,E170,E535	C00362/C00020,C06428/C02075/CE5932/CE5013,C14768/C04742/C14749/C14748/C14769/CE5016/C14778/C14770/C14771/C04805,CE2962,CE5653	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$(5Z,8Z,11Z,14Z,17Z)-Icosape
Glycerophospholipid metabolism	11	19	0.0297454	E420,E62,E296,E55,E452,E432,E653,E449,E599,E496,E562	C06427/C06426,C00577,C00184/C00256/C00186/C01013,C15647,C00795/C00221/C00267/C00031/C00137/C00738/C00095/C00962/C00247/C00984/C00936/C01582/C00159/C02336/C00293/C00124,C14768/C04742/C14749/C14748/C14769/CE5016/C14778/C14770/C14771/C04805,C01595,C027	(9Z,12Z,15Z)-Octadecatrienoic acid; alpha-Linolenic acid; 9,12,15-Octadecatrienoic acid; Linolenate; alpha-Linolenate/(6Z,9Z,12Z)-Octadecatrienoic acid; 6,9,12-Octadecatrienoic acid; gamma-Linolenic acid; Gamolenic acid$D-Glyceraldehyde$Glycerone; Dihydroxyacetone; 1,3-Dihydroxyacetone; 1,3-Dihydroxy-2-
Glycine, serine, alanine and threonine metabolism	-	-	-	-	-	-
Vitamin D3 (cholecalciferol) metabolism	4	4	0.012099824	E153,E79,E216,E41	CE2205,C17335/CE2202,CE2204,C17337/CE2206/CE2203	1alpha,24R,25-trihydroxyvitamin D3$/23S,25,26-trihydroxyvitamin D3$25-hydroxyvitamin D3-26,23-lactone$/24-oxo-1alpha,25-dihydroxyvitamin D3/25-hydroxyvitamin D3-26,23-lactol
Histidine metabolism	-	-	-	-	-	-
Tryptophan metabolism	3	4	0.0148727	E287,E141,E201	C05660,C02470,C05645	5-Methoxyindoleacetate$Xanthurenic acid; Xanthurenate$4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate
Tyrosine metabolism	6	11	0.015796992	E56,E215,E254,E168,E188,E375	C05838/C00166/C02763/C00811,CE4888/C05578,C05583/C05582,C05589/C00788,C01183/C02735/C00483,C00079/CE2172	cis-2-Hydroxycinnamate; 2-Coumarinate/Phenylpyruvate; Phenylpyruvic acid; alpha-Ketohydrocinnamic acid; keto-Phenylpyruvate; 3-Phenyl-2-oxopropanoate/enol-Phenylpyruvate; enol-Phenylpyruvic acid; enol-alpha-Ketohydrocinnamic acid; 2-Hydroxy-3-phenylpropenoate/4-Coumarate; p-Coumaric acid; tra
Vitamin B9 (folate) metabolism	-	-	-	-	-	-
Linoleate metabolism	6	8	0.019830266	E420,E283,E703,E653,E760,E556	C06427/C06426,C14762/C14825/C14826,C14765/CE5526/CE5527,C01595,C14762/C14825/C14826,C14762/C14825/C14826	(9Z,12Z,15Z)-Octadecatrienoic acid; alpha-Linolenic acid; 9,12,15-Octadecatrienoic acid; Linolenate; alpha-Linolenate/(6Z,9Z,12Z)-Octadecatrienoic acid; 6,9,12-Octadecatrienoic acid; gamma-Linolenic acid; Gamolenic acid$13(S)-HODE; (13S)-Hydroxyoctadecadienoic acid; (9Z,11E)-(13S)-13-Hydroxyoctadeca-9,1
Methionine and cysteine metabolism	-	-	-	-	-	-
Glutamate metabolism	-	-	-	-	-	-
Omega-3 fatty acid metabolism	3	3	0.031509957	E70,E761,E420	C16300,C00362/C00020,C06427/C06426	Stearidonic acid; 6,9,12,15-Octadecatetraenoic acid; (6Z,9Z,12Z,15Z)-Octadecatetraenoic acid$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Aden
Sialic acid metabolism	-	-	-	-	-	-
Hexose phosphorylation	-	-	-	-	-	-
Ubiquinone Biosynthesis	-	-	-	-	-	-
Purine metabolism	3	5	0.046718763	E322,E74,E117	C00262,C00312/C00310/C00259/C00181/C00309/C00121,C00294	Hypoxanthine; Purine-6-ol$L-Xylulose; L-threo-Pentulose; L-Lyxulose/D-Xylulose; D-threo-Pentulose; D-Lyxulose/L-Arabinose; L-Arabinopyranose/D-Xylose; Wood sugar/D-Ribulose; D-erythro-2-Pentulose; D-Arabinoketose; D-Arabinulose; D-Riboketose/D-Ribose$Inosine



Heart

SD 4

pathway	*overlap size*	pathway size	*p-value*	overlap Empirical Compounds	overlap features	overlap features name
Fatty acid activation	-	-	-	-	-	-
De novo fatty acid biosynthesis	-	-	-	-	-	-
Xenobiotics metabolism	-	-	-	-	-	-
Fructose and mannose metabolism	1	1	0.005797832	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Nucleotide Sugar Metabolism	1	1	0.005797832	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Linoleate metabolism	-	-	-	-	-	-
Fatty Acid Metabolism	-	-	-	-	-	-
Polyunsaturated fatty acid biosynthesis	1	2	0.011259558	E493	C01530	Octadecanoic acid; Stearate; Stearic acid
Carbon fixation	1	2	0.011259558	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Glycolysis and Gluconeogenesis	1	2	0.011259558	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Hexose phosphorylation	1	2	0.011259558	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Galactose metabolism	1	2	0.011259558	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Arachidonic acid metabolism	-	-	-	-	-	-
Omega-3 fatty acid metabolism	-	-	-	-	-	-
Pyrimidine metabolism	2	9	0.013696328	E428,E101	C00819/C00064/C05100,C00906	D-Glutamine; D-2-Aminoglutaramic acid/L-Glutamine; L-2-Aminoglutaramic acid/3-Ureidoisobutyrate$5,6-Dihydrothymine; Dihydrothymine; 5,6-Dihydro-5-methyluracil
Glycosphingolipid metabolism	-	-	-	-	-	-
Starch and Sucrose Metabolism	1	3	0.020334426	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	1	3	0.020334426	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Saturated fatty acids beta-oxidation	-	-	-	-	-	-
N-Glycan biosynthesis	1	4	0.026384337	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Nitrogen metabolism	1	2	0.026552391	E428	C00819/C00064/C05100	D-Glutamine; D-2-Aminoglutaramic acid/L-Glutamine; L-2-Aminoglutaramic acid/3-Ureidoisobutyrate
Valine, leucine and isoleucine degradation	1	2	0.026552391	E786	C00431/C00183/C00719	5-Aminopentanoate; 5-Aminopentanoic acid; 5-Aminovaleric acid/L-Valine; 2-Amino-3-methylbutyric acid/Betaine; Trimethylaminoacetate; Glycine betaine; N,N,N-Trimethylglycine; Trimethylammonioacetate
Fatty acid oxidation, peroxisome	-	-	-	-	-	-
Aminosugars metabolism	1	5	0.035123099	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Pentose phosphate pathway	1	5	0.035123099	E579	C02965/C05345/C00092/C00085/C00103/C02976/C01171/C01172/C01177/C03735/C00636/C03862/C04006/C01097/C01094/C00668/C03546/C00446/C00275/CE3075	D-Hexose 6-phosphate/beta-D-Fructose 6-phosphate/D-Glucose 6-phosphate; Glucose 6-phosphate; Robison ester/D-Fructose 6-phosphate; D-Fructose 6-phosphoric acid; Neuberg ester/D-Glucose 1-phosphate; alpha-D-Glucose 1-phosphate; Cori ester; D-Glucose alpha-1-phosphate/Fructose 1-phosphate/alph
Arginine and Proline Metabolism	1	3	0.041761197	E428	C00819/C00064/C05100	D-Glutamine; D-2-Aminoglutaramic acid/L-Glutamine; L-2-Aminoglutaramic acid/3-Ureidoisobutyrate
Butanoate metabolism	1	3	0.041761197	E786	C00431/C00183/C00719	5-Aminopentanoate; 5-Aminopentanoic acid; 5-Aminovaleric acid/L-Valine; 2-Amino-3-methylbutyric acid/Betaine; Trimethylaminoacetate; Glycine betaine; N,N,N-Trimethylglycine; Trimethylammonioacetate
Alanine and Aspartate Metabolism	1	3	0.041761197	E428	C00819/C00064/C05100	D-Glutamine; D-2-Aminoglutaramic acid/L-Glutamine; L-2-Aminoglutaramic acid/3-Ureidoisobutyrate

Spleen

SD 4

pathway	*overlap size*	pathway size	*p-value*	overlap Empirical Compounds	overlap features	overlap features name
Glycolysis and Gluconeogenesis	-	-	-	-	-	-
Pentose phosphate pathway	-	-	-	-	-	-
Glycine, serine, alanine and threonine metabolism	-	-	-	-	-	-
Tryptophan metabolism	4	9	0.001260398	E599,E218,E191,E506	C10164/C00253,C02220,C00217/C05938/C00025,C03824	/Nicotinate; Nicotinic acid; Niacin; 3-Pyridinecarboxylic acid$2-Aminomuconate; 2-Aminomuconic acid; o-Aminomuconate$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$2-Aminomuc
Aspartate and asparagine metabolism	3	13	0.032518276	E191,E288,E382	C00217/C05938/C00025,C05145/C01026/C01205/C02356/C00334/C03284,C03287	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$3-Aminoisobutyric acid; 3-Aminoisobutanoate; 3-Amino-2-methylpropanoate/N N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-meth
Fructose and mannose metabolism	-	-	-	-	-	-
Prostaglandin formation from arachidonate	6	11	0.004453407	E340,E34,E382,E90,E54,E512	CE6234/CE5924/CE5929/CE4989/CE5931/CE7093/CE5663/CE5828,C00219,CE5730,C13856,CE5700,C13856	prostaglandin H1///20-OH-10,11-dihydro-leukotriene B4//13,14-dihydro-15-oxo-PGF1/13,14-dihydro- lipoxin A4/$(5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arachidonic acid; cis-5,8,11,14-Eicosatetraenoic acid$$2-Arachidonoylglycerol; 2-Arachidonoyl-sn-glycerol$12-hydroperoxyeicosatetraenoate
Vitamin B3 (nicotinate and nicotinamide) metabolism	3	6	0.004705487	E599,E191,E350	C10164/C00253,C00217/C05938/C00025,C01185	/Nicotinate; Nicotinic acid; Niacin; 3-Pyridinecarboxylic acid$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$Nicotinate D-ribonucleotide; beta-Nicotinate D-ribonucleotide; Nicotinate rib
Pyruvate Metabolism	-	-	-	-	-	-
Butanoate metabolism	1	2	0.019662213	E491	C00431/C00183/C00719	5-Aminopentanoate; 5-Aminopentanoic acid; 5-Aminovaleric acid/L-Valine; 2-Amino-3-methylbutyric acid/Betaine; Trimethylaminoacetate; Glycine betaine; N,N,N-Trimethylglycine; Trimethylammonioacetate
Ascorbate (Vitamin C) and Aldarate Metabolism	-	-	-	-	-	-
Galactose metabolism	-	-	-	-	-	-
Polyunsaturated fatty acid biosynthesis	1	1	0.007730443	E201	C01530	Octadecanoic acid; Stearate; Stearic acid
Valine, leucine and isoleucine degradation	1	3	0.027728762	E491	C00431/C00183/C00719	5-Aminopentanoate; 5-Aminopentanoic acid; 5-Aminovaleric acid/L-Valine; 2-Amino-3-methylbutyric acid/Betaine; Trimethylaminoacetate; Glycine betaine; N,N,N-Trimethylglycine; Trimethylammonioacetate
Pyrimidine metabolism	4	16	0.014284514	E309,E191,E287,E288	C00299,C00217/C05938/C00025,C00380,C05145/C01026/C01205/C02356/C00334/C03284	Uridine$D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$Cytosine$3-Aminoisobutyric acid; 3-Aminoisobutanoate; 3-Amino-2-methylpropanoate/N N-Dimethylglycine; Dimethylglycine/(R
Lysine metabolism	-	-	-	-	-	-
Carbon fixation	-	-	-	-	-	-
Purine metabolism	-	-	-	-	-	-
Fatty acid activation	4	7	0.010839425	E576,E192,E14,E502	C00712/C01712,C00249,C01595,tettet6	(9Z)-Octadecenoic acid; (Z)-Octadec-9-enoic acid; Oleate; Oleic acid/(9E)-Octadecenoic acid; 9-Octadecenoic acid, (E)-; (E)-Oleic acid; D9-trans-Octadecenoic acid; 9-trans-Octadecenoic acid; trans-D9-Octadecenoic acid; trans-9-Octadecenoic acid; trans-Elaidic acid; trans-Oleic acid; Elaidic acid; Acide elaidique; Elai
TCA cycle	-	-	-	-	-	-
Propanoate metabolism	-	-	-	-	-	-
Glycerophospholipid metabolism	-	-	-	-	-	-
Urea cycle/amino group metabolism	3	10	0.017729603	E191,E288,E382	C00217/C05938/C00025,C05145/C01026/C01205/C02356/C00334/C03284,C03287	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$3-Aminoisobutyric acid; 3-Aminoisobutanoate; 3-Amino-2-methylpropanoate/N N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-meth
Fatty Acid Metabolism	3	5	0.018821948	E288,E14,E192	3ohxccoa,C01595,C00249	3-Oxohexacosyl-CoA$Linoleate; Linoleic acid; (9Z,12Z)-Octadecadienoic acid; 9-cis,12-cis-Octadecadienoate; 9-cis,12-cis-Octadecadienoic acid$Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid
De novo fatty acid biosynthesis	5	12	0.025628098	E34,E576,E192,E14,E332	C00219,C00712/C01712,C00249,C01595,C00712	(5Z,8Z,11Z,14Z)-Icosatetraenoic acid; Arachidonate; Arachidonic acid; cis-5,8,11,14-Eicosatetraenoic acid$(9Z)-Octadecenoic acid; (Z)-Octadec-9-enoic acid; Oleate; Oleic acid/(9E)-Octadecenoic acid; 9-Octadecenoic acid, (E)-; (E)-Oleic acid; D9-trans-Octadecenoic acid; 9-trans-Octadecenoic acid; trans-D9-Octadec
Drug metabolism - cytochrome P450	-	-	-	-	-	-
Glutamate metabolism	2	7	0.048903453	E191,E288	C00217/C05938/C00025,C05145/C01026/C01205/C02356/C00334/C03284	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$3-Aminoisobutyric acid; 3-Aminoisobutanoate; 3-Amino-2-methylpropanoate/N N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-meth
Glutathione Metabolism	-	-	-	-	-	-
Putative anti-Inflammatory metabolites formation from EPA	-	-	-	-	-	-
Histidine metabolism	-	-	-	-	-	-
Arginine and Proline Metabolism	-	-	-	-	-	-
Beta-Alanine metabolism	2	6	0.035291152	E191,E288	C00217/C05938/C00025,C05145/C01026/C01205/C02356/C00334/C03284	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$3-Aminoisobutyric acid; 3-Aminoisobutanoate; 3-Amino-2-methylpropanoate/N N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-meth
Trihydroxycoprostanoyl-CoA beta-oxidation	-	-	-	-	-	-
Glycosphingolipid metabolism	3	6	0.033862701	E192,E515,E250	C00249,C01120,C12144	Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid$Sphinganine 1-phosphate; Dihydrosphingosine 1-phosphate$Phytosphingosine; 4-D-Hydroxysphinganine
Aminosugars metabolism	2	6	0.035291152	E191,E181	C00217/C05938/C00025,C00128	D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde/L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate$CMP-N-acetylneuraminate
Fatty acid oxidation, peroxisome	-	-	-	-	-	-
Parathio degradation	1	1	0.0392404	E40	C00870	4-Nitrophenol; p-Nitrophenol; PNP; Niphen; 4-Hydroxynitrobenzene

Kidney

SD 4

pathway	*overlap size*	pathway size	*p-value*	overlap Empirical Compounds	overlap features	overlap features name
Beta-Alanine metabolism	6	6	0.001092345	E322,E672,E402,E56,E422,E356	C05145/C01026/C01205/C02356/C00334/C03284,C00025/C00217/C05938,C00222/C00022,C00402/C00049,C00184/C00256/C00186/C01013,C00135	3-Aminoisobutyric acid; 3-Aminoisobutanoate; 3-Amino-2-methylpropanoate/N N-Dimethylglycine; Dimethylglycine/(R)-3-Amino-2-methylpropanoate; D-3-Amino-isobutanoate/(S)-2-Aminobutanoate; (S)-2-Aminobutanoic acid; (S)-2-Aminobutyric acid/4-Aminobutanoate; 4-Aminobutanoic acid; 4-Aminobuty
Valine, leucine and isoleucine degradation	2	3	7.56E-04	E184,E205	C00431/C00183/C00719,C01188/C06001/C01089/C03197/C00989/C05984	5-Aminopentanoate; 5-Aminopentanoic acid; 5-Aminovaleric acid/L-Valine; 2-Amino-3-methylbutyric acid/Betaine; Trimethylaminoacetate; Glycine betaine; N,N,N-Trimethylglycine; Trimethylammonioacetate$3-Hydroxy-2-methylpropanoate; 3-Hydroxyisobutyrate; 3-Hydroxyisobutyric acid/(S)-3-Hydroxyisobu
Butanoate metabolism	8	10	0.001512478	E442,E286,E485,E672,E402,E322,E206,E745	C00362/C00020,C00266/C00033,C00042/C02170,C00025/C00217/C05938,C00222/C00022,C05145/C01026/C01205/C02356/C00334/C03284,C03087,C06001/C01089/C03197/C00989/C05984	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$Glycolaldehyde; Hydroxyace
Tryptophan metabolism	2	4	0.001764558	E79,E202	C02470,C05645	Xanthurenic acid; Xanthurenate$4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate
Pyruvate Metabolism	5	5	0.002268717	E402,E289,E128,E286,E422	C00222/C00022,C00149,CE0737/C00546/C00511,C00266/C00033,C00184/C00256/C00186/C01013	3-Oxopropanoate; Malonate semialdehyde/Pyruvate; Pyruvic acid; 2-Oxopropanoate; 2-Oxopropanoic acid; Pyroracemic acid$(S)-Malate; L-Malate; L-Apple acid; L-Malic acid; L-2-Hydroxybutanedioic acid$malonic dialdehyde/Methylglyoxal; Pyruvaldehyde; Pyruvic aldehyde; 2-Ketopropionaldehyde; 2-Oxopro
Aspartate and asparagine metabolism	10	15	0.00268885	E442,E322,E465,E542,E672,E56,E286,E486,E745,E233	C00362/C00020,C05145/C01026/C01205/C02356/C00334/C03284,C02266/C01087/C02630/C03196,C04281/C04282/C01879,C00025/C00217/C05938,C00402/C00049,C00266/C00033,C00097,C06001/C01089/C03197/C00989/C05984,C02238	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$3-Aminoisobutyric acid; 3-A
Ascorbate (Vitamin C) and Aldarate Metabolism	4	8	0.002856903	E636,E242,E203,E41	C02045,C01620,C00257/C00800,CE5985	$$D-Gluconic acid; D-Gluconate; D-gluco-Hexonic acid/L-Gulonate; L-Gulonic acid; Gulonate; Gulonic acid$
Alanine and Aspartate Metabolism	6	7	0.003193009	E442,E286,E672,E402,E56,E695	C00362/C00020,C00266/C00033,C00025/C00217/C05938,C00222/C00022,C00402/C00049,C00122	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$Glycolaldehyde; Hydroxyace
Methionine and cysteine metabolism	8	11	0.003361062	E442,E497,E286,E672,E402,E568,E486,E30	C00362/C00020,C00491,C00266/C00033,C00025/C00217/C05938,C00222/C00022,C00245,C00097,C00302	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$L-Cystine; L-Dicysteine; L-al
Vitamin B9 (folate) metabolism	-	-	-	-	-	-
Histidine metabolism	4	4	0.005965885	E672,E442,E356,E402	C00025/C00217/C05938,C00362/C00020,C00135,C00222/C00022	L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate/D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde$dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/A
Vitamin B3 (nicotinate and nicotinamide) metabolism	-	-	-	-	-	-
Glycerophospholipid metabolism	4	19	0.036467524	E537,E538,E261,E168	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C00055,C00266/C00033,C02737	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H
Pentose phosphate pathway	3	7	0.011427611	E537,E203,E430	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C00257/C00800,C00312/C00310/C00508/C00259/C00181/C00309/C00121	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H
Sialic acid metabolism	3	8	0.016049072	E538,E537,E168	C00055,C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C02737	CMP; Cytidine-5'-monophosphate; Cytidylic acid$D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios
Chondroitin sulfate degradation	2	3	0.014704647	E537,E430	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C00312/C00310/C00508/C00259/C00181/C00309/C00121	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H
Glycosphingolipid biosynthesis - globoseries	2	3	0.014704647	E538,E537	C00055,C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124	CMP; Cytidine-5'-monophosphate; Cytidylic acid$D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios
Glyoxylate and Dicarboxylate Metabolism	2	3	0.014704647	E261,E430	C00266/C00033,C00312/C00310/C00508/C00259/C00181/C00309/C00121	Glycolaldehyde; Hydroxyacetaldehyde/Acetate; Acetic acid; Ethanoic acid; Glacial acetic acid$L-Xylulose; L-threo-Pentulose; L-Lyxulose/D-Xylulose; D-threo-Pentulose; D-Lyxulose/L-Ribulose; L-erythro-Pentulose; L-Arabinoketose; L-Arabinulose; L-Riboketose/L-Arabinose; L-Arabinopyranose/D-Xylose; Wood sug
Glycine, serine, alanine and threonine metabolism	8	13	0.015376859	E442,E322,E672,E402,E128,E286,E143,E422	C00362/C00020,C05145/C01026/C01205/C02356/C00334/C03284,C00025/C00217/C05938,C00222/C00022,CE0737/C00546/C00511,C00266/C00033,C00258,C00184/C00256/C00186/C01013	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$3-Aminoisobutyric acid; 3-A
Biopterin metabolism	-	-	-	-	-	-
Arginine and Proline Metabolism	6	9	0.020250399	E485,E542,E672,E402,E56,E695	C00042/C02170,C04281/C04282/C01879,C00025/C00217/C05938,C00222/C00022,C00402/C00049,C00122	Succinate; Succinic acid; Butanedioic acid; Ethylenesuccinic acid/Methylmalonate; Methylmalonic acid$L-1-Pyrroline-3-hydroxy-5-carboxylate; 3-Hydroxy-L-1-pyrroline-5-carboxylate; (3R,5S)-1-Pyrroline-3-hydroxy-5-carboxylate/1-Pyrroline-4-hydroxy-2-carboxylate/5-Oxoproline; Pyroglutamic acid; 5-Pyrrolido
Aminosugars metabolism	6	9	0.020250399	E286,E672,E23,E402,E436,E706	C00266/C00033,C00025/C00217/C05938,C03410,C00222/C00022,C04501/C04256/C04257/C00357/C06376,C00055	Glycolaldehyde; Hydroxyacetaldehyde/Acetate; Acetic acid; Ethanoic acid; Glacial acetic acid$L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate/D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde$N-Glycolyl-neuraminate; N-Glycolylneuram
Phosphatidylinositol phosphate metabolism	3	9	0.020586505	E538,E537,E261	C00055,C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C00266/C00033	CMP; Cytidine-5'-monophosphate; Cytidylic acid$D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios
Glutathione Metabolism	3	3	0.020754558	E672,E542,E486	C00025/C00217/C05938,C04281/C04282/C01879,C00097	L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate/D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde$L-1-Pyrroline-3-hydroxy-5-carboxylate; 3-Hydroxy-L-1-pyrroline-5-carboxylate; (3R,5S)-1-Pyrroline-3-hydroxy-5-carboxylate/1-Pyrroline-4-
Vitamin B1 (thiamin) metabolism	3	3	0.020754558	E442,E402,E424	C00362/C00020,C00222/C00022,C01081	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$3-Oxopropanoate; Malonat
Glycosphingolipid metabolism	-	-	-	-	-	-
Selenoamino acid metabolism	-	-	-	-	-	-
Heparan sulfate degradation	2	4	0.022351063	E537,E430	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C00312/C00310/C00508/C00259/C00181/C00309/C00121	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H
Glycosphingolipid biosynthesis - ganglioseries	2	4	0.022351063	E537,E538	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C00055	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H
Glycolysis and Gluconeogenesis	5	7	0.022519116	E442,E402,E289,E286,E422	C00362/C00020,C00222/C00022,C00149,C00266/C00033,C00184/C00256/C00186/C01013	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$3-Oxopropanoate; Malonat
Glutamate metabolism	4	5	0.023863541	E672,E402,E322,E485	C00025/C00217/C05938,C00222/C00022,C05145/C01026/C01205/C02356/C00334/C03284,C00042/C02170	L-Glutamate; L-Glutamic acid; L-Glutaminic acid; Glutamate/D-Glutamate; D-Glutamic acid; D-Glutaminic acid; D-2-Aminoglutaric acid/L-4-Hydroxyglutamate semialdehyde$3-Oxopropanoate; Malonate semialdehyde/Pyruvate; Pyruvic acid; 2-Oxopropanoate; 2-Oxopropanoic acid; Pyroracemic acid$3-Aminoiso
Purine metabolism	8	14	0.02487186	E442,E672,E402,E56,E707,E410,E345,E695	C00362/C00020,C00025/C00217/C05938,C00222/C00022,C00402/C00049,C01762,C00385,C00294,C00122	dGMP; 2'-Deoxyguanosine 5'-monophosphate; 2'-Deoxyguanosine 5'-phosphate; Deoxyguanylic acid; Deoxyguanosine monophosphate/AMP; Adenosine 5'-monophosphate; Adenylic acid; Adenylate; 5'-AMP; 5'-Adenylic acid; 5'-Adenosine monophosphate; Adenosine 5'-phosphate$L-Glutamate; L-Glutamic ac
Vitamin B6 (pyridoxine) metabolism	1	2	0.025544072	E278	C00250	Pyridoxal
Propanoate metabolism	1	2	0.025712125	E205	C01188/C06001/C01089/C03197/C00989/C05984	3-Hydroxy-2-methylpropanoate; 3-Hydroxyisobutyrate; 3-Hydroxyisobutyric acid/(S)-3-Hydroxyisobutyrate/(R)-3-Hydroxybutanoate; (R)-3-Hydroxybutanoic acid; (R)-3-Hydroxybutyric acid/(S)-3-Hydroxybutanoate/4-Hydroxybutanoic acid; 4-Hydroxybutanoate; 4-Hydroxybutyric acid/2-Hydroxybutanoic acid; 2
Leukotriene metabolism	-	-	-	-	-	-
Pentose and Glucuronate Interconversions	2	5	0.033358541	E203,E430	C00257/C00800,C00312/C00310/C00508/C00259/C00181/C00309/C00121	D-Gluconic acid; D-Gluconate; D-gluco-Hexonic acid/L-Gulonate; L-Gulonic acid; Gulonate; Gulonic acid$L-Xylulose; L-threo-Pentulose; L-Lyxulose/D-Xylulose; D-threo-Pentulose; D-Lyxulose/L-Ribulose; L-erythro-Pentulose; L-Arabinoketose; L-Arabinulose; L-Riboketose/L-Arabinose; L-Arabinopyranose/D-Xylose;
Urea cycle/amino group metabolism	-	-	-	-	-	-
Parathio degradation	-	-	-	-	-	-
Ubiquinone Biosynthesis	-	-	-	-	-	-
Hexose phosphorylation	-	-	-	-	-	-
N-Glycan biosynthesis	2	6	0.047727082	E537,E538	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124,C00055	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H
N-Glycan Degradation	1	1	0.048147215	E537	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H
Proteoglycan biosynthesis	1	1	0.048147215	E261	C00266/C00033	Glycolaldehyde; Hydroxyacetaldehyde/Acetate; Acetic acid; Ethanoic acid; Glacial acetic acid
Keratan sulfate degradation	1	1	0.048147215	E537	C00795/C00221/C00095/C00267/C00137/C00738/C00962/C00247/C00984/C00031/C00936/C01582/C00159/C02336/C00293/C00124	D-Tagatose; lyxo-Hexulose/beta-D-Glucose/D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose/alpha-D-Glucose/myo-Inositol; D-myo-Inositol; 1D-myo-Inositol; L-myo-Inositol; 1L-myo-Inositol; meso-Inositol; Inositol; Dambose; Cyclohexitol; Meat sugar; Bios I/D-Hexose/beta-D-Galactose/L-Sorbose; L-xylo-H

Heart

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds		overlap features
Fatty acid activation	6	15	1.68E-04	E313,E19,E718,E557,E333,E764	C06427/C06426,C03242,C00249,C06427/C06426,C00249,C01595	[illegible]
De novo fatty acid biosynthesis	7	23	6.72E-04	E313,E19,E718,E165,E557,E333,E764	C06427/C06426,C03242,C00249,C06429,C06427/C06426,C00249,C01595	[illegible]
Xenobiotics metabolism	3	5	0.0022687	E333,E18,E718	C00249,C00829,C00249	[illegible]
Fructose and mannose metabolism	-	-	-	-	-	-
Nucleotide Sugar Metabolism	-	-	-	-	-	-
Linoleate metabolism	4	12	0.0058819	E313,E764,E926,E557	C06427/C06426,C01595,C14762/C14825/C14826,C06427/C06426	[illegible]
Fatty Acid Metabolism	3	8	0.0086547	E333,E764,E718	C00249,C01595,C00249	[illegible]
Polyunsaturated fatty acid biosynthesis	-	-	-	-	-	-
Carbon fixation	-	-	-	-	-	-
Glycolysis and Gluconeogenesis	-	-	-	-	-	-
Hexose phosphorylation	-	-	-	-	-	-
Galactose metabolism	-	-	-	-	-	-
Arachidonic acid metabolism	3	9	0.0120998	E901,E313,E557	leuktrE4,C06427/C06426,C06427/C06426	[illegible]
Omega-3 fatty acid metabolism	2	4	0.012688	E313,E557	C06427/C06426,C06427/C06426	[illegible]
Pyrimidine metabolism	-	-	-	-	-	-
Glycosphingolipid metabolism	4	16	0.0151248	E333,E277,E48,E718	C00249,C00836,C01747,C00249	[illegible]
Starch and Sucrose Metabolism	-	-	-	-	-	-
Glycosylphosphatidylinositol(GPI)-anchor biosynthesis	-	-	-	-	-	-
Saturated fatty acids beta-oxidation	2	5	0.0211747	E333,E718	C00249,C00249	[illegible]
N-Glycan biosynthesis	-	-	-	-	-	-
Nitrogen metabolism	-	-	-	-	-	-
Valine, leucine and isoleucine degradation	-	-	-	-	-	-
Fatty acid oxidation, peroxisome	1	1	0.0291572	E509	ttccoa/lgnccoa/CE2257	[illegible]
Aminosugars metabolism	-	-	-	-	-	-
Pentose phosphate pathway	-	-	-	-	-	-
Arginine and Proline Metabolism	-	-	-	-	-	-
Butanoate metabolism	-	-	-	-	-	-
Alanine and Aspartate Metabolism	-	-	-	-	-	-

Spleen

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds		overlap features
Glycolysis and Gluconeogenesis	7	7	5.88E-04	E386,E241,E605,E649,E313,E439,E131	[illegible]	[illegible]
Pentose phosphate pathway	7	9	6.72E-04	E314,E496,E89,E600,E607,E501,E589	[illegible]	[illegible]
Glycine, serine, alanine and threonine metabolism	8	10	7.56E-04	E211,E462,E26,E399,E459,E129,E70,E19	CE1554,C00025,C00431/C00183/C00719,C00248,C01419,C00256/C00186/C00184/C01013/C00577,C00051,CE0469	[illegible]
Tryptophan metabolism	7	9	0.0088228	E386,E203,E64,E672,E218,E303,E439	C00020/C00362,C02220,C00051,C10164/C00253,C03824,C05938/C00217/C00025,C00795/C00221/C00267/C00031/C00137/C00738/C00095/C00962/C00247/C01582/C00984/C00936/C00159/C02336/C00293/C00124	[illegible]
Aspartate and asparagine metabolism	6	7	0.0014285	E564,E462,E300,E384,E459,E70	C01239,C00025,C00217/C05938/C00302,C00169,C01419,C00051	[illegible]
Fructose and mannose metabolism	5	6	0.0035291	E600,E333,E501,E496,E285	[illegible]	[illegible]
Prostaglandin formation from arachidonate	-	-	-	-	-	-
Vitamin B3 (nicotinate and nicotinamide) metabolism	5	6	0.0156289	E386,E506,E303,E581,E672	C00020/C00362,C01185,C05938/C00217/C00025,C01101/C03736/C00442/C00199,C10164/C00253	[illegible]
Pyruvate Metabolism	5	5	0.0049576	E64,E313,E606,E605,E131	C00051,C00661/C00111/C00118,C00546/CE0737/C00511,C00149,C00256/C00186/C00184/C01013	[illegible]
Butanoate metabolism	6	7	0.0068062	E386,E405,E674,E731,E141,E303	C00020/C00362,C00042/C02170,C00164/C00109/C00349/C06002/C00232,C06001/C01089/C03197/C00989/C05984,C06144,C05938/C00217/C00025	[illegible]
Ascorbate (Vitamin C) and Aldarate Metabolism	6	7	0.0068062	E253,E64,E639,E172,E442,E607	C00311/C00158/C04575,C00051,C02045,C02147,C00818,C01620	[illegible]
Galactose metabolism	6	7	0.0068062	E229,E241,E649,E222,E313,E439	[illegible]	[illegible]
Polyunsaturated fatty acid biosynthesis	-	-	-	-	-	-
Valine, leucine and isoleucine degradation	3	3	0.0085707	E26,E399,E462	C00431/C00183/C00719,C00248,C00025	[illegible]
Pyrimidine metabolism	3	3	0.0085707	E518,E462,E384	C05345/C00092/C00085/C00103/C01172/C01177/C00636/C03862/C04006/C01097/C01094/C03546/C00446/C00275,CE3075,C00025,C00169	[illegible]
Lysine metabolism	3	3	0.0085707	E399,E323,E462	C00248,C00318,C00025	[illegible]
Carbon fixation	4	5	0.0097471	E333,E607,E501,E496	[illegible]	[illegible]
Purine metabolism	4	5	0.0102512	E538,E364,E130,E462	C03373,C00262,C00385,C00025	[illegible]
Fatty acid activation	-	-	-	-	-	-
TCA cycle	4	4	0.0120998	E405,E605,E328,E253	C00042/C02170,C00149,C00122,C00311/C00158/C04575	[illegible]
Propanoate metabolism	4	4	0.0120998	E386,E731,E674,E131	[illegible]	[illegible]
Glycerophospholipid metabolism	9	19	0.0131922	E45,E496,E590,E299,E241,E112,E600,E285,E501	[illegible]	[illegible]
Urea cycle/amino group metabolism	-	-	-	-	-	-
Fatty Acid Metabolism	-	-	-	-	-	-
De novo fatty acid biosynthesis	-	-	-	-	-	-
Drug metabolism - cytochrome P450	3	4	0.0292412	E576,E461,E244	CE2173/C16586,C16662,C07501	[illegible]
Glutamate metabolism	3	4	0.0303336	E70,E462,E384	C00051,C00025,C00169	[illegible]
Glutathione Metabolism	3	4	0.0303336	E70,E459,E462	C00051,C01419,C00025	[illegible]
Putative anti-Inflammatory metabolites formation from EPA	2	2	0.031762	E70,E462	C00051,C00025	[illegible]
Histidine metabolism	2	2	0.031762	E70,E462	C00051,C00025	[illegible]
Arginine and Proline Metabolism	2	2	0.031762	E300,E462	C00217/C05938/C00302,C00025	[illegible]
Beta-Alanine metabolism	2	2	0.031762	E129,E462	C00256/C00186/C00184/C01013/C00577,C00025	[illegible]
Trihydroxycoprostanoyl-CoA beta-oxidation	2	2	0.031762	E215,E100	CE5169,CE5168	[illegible]
Glycosphingolipid metabolism	-	-	-	-	-	-
Aminosugars metabolism	-	-	-	-	-	-
Fatty acid oxidation, peroxisome	2	2	0.0373918	E492,E474	CE2245/CE5159/hmcoa,C00042/C02170	[illegible]
Parathio degradation	-	-	-	-	-	-

Kidney

pathway	overlap size	pathway size	p-value	overlap Empirical Compounds		overlap features
Beta-Alanine metabolism	6	6	5.88E-04	E713,E472,E581,E71,E539,E648	[illegible]	[illegible]
Valine, leucine and isoleucine degradation	-	-	-	-	-	-
Butanoate metabolism	-	-	-	-	-	-
Tryptophan metabolism	3	10	0.0233594	E498,E461,E524	C03824,C02220,C10164/C00253	[illegible]
Pyruvate Metabolism	-	-	-	-	-	-
Aspartate and asparagine metabolism	-	-	-	-	-	-
Ascorbate (Vitamin C) and Aldarate Metabolism	6	8	0.0073103	E716,E281,E505,E627,E13,E43	glac/C00072/C02670,CE5985,C00311/C00158/C04575,C01620,C02045,C00818	[illegible]
Alanine and Aspartate Metabolism	-	-	-	-	-	-
Methionine and cysteine metabolism	1	3	0.022015	E146	C00065/C00740	[illegible]
Vitamin B9 (folate) metabolism	1	1	0.0055458	E146	C00065/C00740	[illegible]
Histidine metabolism	3	4	0.0468028	E713,E71,E472	C00217/C05938/C00025,C00222/C00022,C00135	[illegible]
Vitamin B3 (nicotinate and nicotinamide) metabolism	3	6	0.0073103	E457,E524,E547	C00049/C00402,C10164/C00253,C01185	[illegible]
Glycerophospholipid metabolism	2	10	0.0076464	E146,E155	C00065/C00740,C04598	[illegible]
Pentose phosphate pathway	-	-	-	-	-	-
Sialic acid metabolism	1	2	0.0133602	E146	C00065/C00740	[illegible]
Chondroitin sulfate degradation	-	-	-	-	-	-
Glycosphingolipid biosynthesis - globoseries	-	-	-	-	-	-
Glyoxylate and Dicarboxylate Metabolism	-	-	-	-	-	-
Glycine, serine, alanine and threonine metabolism	1	5	0.0362154	E146	C00065/C00740	[illegible]
Biopterin metabolism	2	4	0.0186539	E714,E460	C00079/CE2172,C00082/CE2174	[illegible]
Arginine and Proline Metabolism	-	-	-	-	-	-
Aminosugars metabolism	-	-	-	-	-	-
Phosphatidylinositol phosphate metabolism	-	-	-	-	-	-
Glutathione Metabolism	-	-	-	-	-	-
Vitamin B1 (thiamin) metabolism	-	-	-	-	-	-
Glycosphingolipid metabolism	1	3	0.022015	E146	C00065/C00740	[illegible]
Selenoamino acid metabolism	1	3	0.022015	E146	C00065/C00740	[illegible]
Heparan sulfate degradation	-	-	-	-	-	-
Glycosphingolipid biosynthesis - ganglioseries	-	-	-	-	-	-
Glycolysis and Gluconeogenesis	-	-	-	-	-	-
Glutamate metabolism	-	-	-	-	-	-
Purine metabolism	-	-	-	-	-	-
Vitamin B6 (pyridoxine) metabolism	-	-	-	-	-	-
Propanoate metabolism	-	-	-	-	-	-
Leukotriene metabolism	1	4	0.0298294	E366	CE4995	[illegible]
Pentose and Glucuronate Interconversions	-	-	-	-	-	-
Urea cycle/amino group metabolism	3	12	0.0373918	E26,E457,E268	C05589/C00788,C00049/C00402,C01026/C01205/C02356/C00334/C03284/C05145	[illegible]
Parathio degradation	1	1	0.041257	E238	C00870	[illegible]
Ubiquinone Biosynthesis	1	2	0.0457104	E334	C05838/C00166/C02763/C00811	[illegible]
Hexose phosphorylation	1	2	0.0457104	E334	C05838/C00166/C02763/C00811	[illegible]
N-Glycan biosynthesis	-	-	-	-	-	-
N-Glycan Degradation	-	-	-	-	-	-
Proteoglycan biosynthesis	-	-	-	-	-	-
Keratan sulfate degradation	-	-	-	-	-	-

-Hexose 6-phosphate/beta-D-Fructose 6-phosp
r; Glucose 6-phosphate; Robison ester/D-Hexos

Hexose/D-Fructose; Levulose; Fr

itol 1,3-bisphosphate; myo-In

tyric acid$3-Butynoate$L-4-Hydroxygl

-Inositol 1-phosphate; D-myo-Inositol 1-phospha

nositol 4-phosphate/alpha-D-Galactose 1-phosphate; alpha-D

sphate/Fructose 1-phosphate/alpha-D-Hexose 1-p

(S)-Lactate; L-Lactate; L-Lactic ac
Hydroxyeicosatetraenoic aci

id; gamma-Aminobutyri