Supporting Information

Metabolic Profiling of a Porcine Combat Trauma-Injury Model Using NMR and Multi-Mode LC-MS Metabolomics—A Preliminary Study

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Table S1. Fold-change comparison of significant features from NMR binned data ($p < 0.05$).

Chemical shift (ppm)	Multiplicity	Molecule	Assignment	FC SHAM Mean (SD)	FC TRAUMA Mean (SD)
0.75	m	Cholesterol	C26 and C27	1.01 (0.22)	0.51 (0.1)
0.77	m	Cholesterol	C26 and C27	1.01 (0.19)	0.49 (0.07)
0.79	m	Cholesterol	C26 and C27	1.01 (0.19)	0.48 (0.05)
0.81	m	Lipids (Mainly LDL)	$CH_3(CH_2)_n$	1.04 (0.25)	0.49 (0.06)
0.83	m	Lipids (Mainly LDL)	$CH_3(CH_2)_n$	1.01 (0.19)	0.47 (0.06)
0.85	m	Lipids (Mainly VLDL)	$CH_3CH_2CH_2C=$	0.95 (0.15)	0.46 (0.06)
0.87	m	Lipids (Mainly VLDL)	$CH_3CH_2CH_2C=$	0.96 (0.16)	0.49 (0.06)
0.89	m	Lipids (Mainly VLDL)	$CH_3CH_2CH_2C=$	0.98 (0.14)	0.48 (0.06)
0.91		Cholesterol	C21	0.96 (0.17)	0.53 (0.09)
0.93	m	Lipids	δ-CH_3/CH_3CH_2	1.02 (0.19)	0.59 (0.09)
0.95	d	Leucine/Lipids	δ-CH_3/CH_3CH_2	1.02 (0.17)	0.76 (0.14)
1.19	m	Lipids	$CH_3CH_2CH_2$	0.91 (0.18)	0.47 (0.04)
1.21	m	Lipids	$CH_3CH_2CH_2$	1 (0.18)	0.49 (0.08)
1.23	m	Lipids	$CH_3CH_2CH_2$	0.96 (0.14)	0.48 (0.07)
1.25	m	Lipids (Mainly LDL)	$(CH_2)_n$	0.96 (0.14)	0.51 (0.06)
1.27	m	Lipids	$CH_3CH_2(CH_2)_n$	1.05 (0.17)	0.52 (0.05)
1.29	m	Lipids (Mainly VLDL)	$CH_2CH_2CH_2CO$	0.98 (0.15)	0.51 (0.06)
1.39		Unknown		0.9 (0.18)	0.45 (0.11)
1.41		Unknown		0.94 (0.15)	0.44 (0.1)
1.43		Unknown		0.91 (0.15)	0.53 (0.17)

1.57	m	Lipids (mainly VLDL)	CH_2CH_2CO	1.09 (0.3)	0.47 (0.08)
1.59	m	Lipids/Citrulline	CH_2CH_2CO/γ-CH_2	1.03 (0.22)	0.43 (0.08)
1.61	m	Lipids/Citrulline	CH_2CH_2CO/γ-CH_2	1.01 (0.21)	0.41 (0.09)
1.65	m	Arginine	γ-CH_2	1.04 (0.25)	0.51 (0.07)
1.67	m	Arginine/Lipids	γ-CH_2/CH_2CH_2C=C	1.02 (0.19)	0.54 (0.07)
1.69	m	Lysine/Lipids	δ-CH_2/CH_2CH_2C=C	1.02 (0.19)	0.63 (0.11)
1.71	m	Leucine/Lipids	β-CH_2, γ-CH/CH_2CH_2C=C	1.03 (0.18)	0.75 (0.12)
1.73	m	Leucine/Lipids	β-CH_2, γ-CH/CH_2CH_2C=C	1.01 (0.13)	0.76 (0.12)
1.93	s	Acetate	CH_3	0.9 (0.12)	0.5 (0.17)
1.95	m	Lipids	CH_2C=C	1.08 (0.26)	0.47 (0.07)
1.97	m	Lipids	CH_2C=C	1.04 (0.23)	0.52 (0.08)
1.99	m	Lipids	CH_2C=C	1.03 (0.19)	0.54 (0.07)
2.01	m	Lipids	CH_2C=C	1.01 (0.17)	0.53 (0.06)
2.03	s	Glycoproteins (N-acetyl)	$NHCOCH_3$	1.08 (0.3)	0.51 (0.07)
2.05	m	Proline	half β-CH_2	0.92 (0.15)	0.43 (0.08)
2.07	s	Glycoproteins (N-acetyl)	$OCOCH_3$	0.99 (0.18)	0.49 (0.08)
2.09	m	Glutamine	half γ-CH_2	0.97 (0.27)	0.52 (0.11)
2.25	m	Valine/Lipids	β-CH/CH_2CO	1.05 (0.23)	0.54 (0.1)
2.27	m	Valine/Lipids	β-CH/CH_2CO	1 (0.18)	0.56 (0.11)
2.29	m	Valine/Lipids	β-CH/CH_2CO	0.97 (0.1)	0.5 (0.14)
2.31	m	Valine/Lipids	β-CH/CH_2CO	0.97 (0.11)	0.48 (0.13)
2.33	m	Glutamate	half γ-CH_2	1.01 (0.2)	0.68 (0.13)
2.67	d/m	Citrate/Lipids	half CH_2/C=CCH_2C=C	1.04 (0.15)	0.54 (0.18)
2.69	d/m	Citrate/Lipids	half CH_2/C=CCH_2C=C	1.01 (0.16)	0.56 (0.13)
2.71	d/m	Citrate/Lipids	half CH_2/C=CCH_2C=C	0.94 (0.19)	0.49 (0.15)
2.73	m	Lipids	half CH_2/C=CCH_2C=C	1.06 (0.3)	0.5 (0.11)
2.75	m	Lipids	half CH_2/C=CCH_2C=C	1.03 (0.28)	0.48 (0.11)
2.93	t	Albumin (lysyl)	ϵ-CH_2	0.97 (0.26)	0.59 (0.13)
2.95	t	Albumin (lysyl)	ϵ-CH_2	0.99 (0.23)	0.51 (0.11)
2.97	t	Albumin (lysyl)	ϵ-CH_2	0.99 (0.21)	0.49 (0.11)
2.99	t	Albumin (lysyl)	ϵ-CH_2	0.97 (0.19)	0.48 (0.1)
3.01	t	Albumin (lysyl)	ϵ-CH_2	0.98 (0.19)	0.55 (0.12)
3.07	dd	Tyrosine	half β-CH_2	0.96 (0.25)	0.5 (0.11)
3.11	dd	Phenylalanine	half β-CH_2	1.04 (0.3)	0.6 (0.19)
3.21	s	Choline	$N(CH_3)_3$	1.05 (0.24)	0.55 (0.07)
3.27	s/dd	Betaine/Glucose	$N(CH_3)_3/H_2$ of β-Glucose	0.98 (0.14)	0.52 (0.19)
3.55	s/dd	Glycine/Glucose	CH_2/H_2 of α-Glucose	1.00 (0.17)	0.75 (0.11)
3.57	d/m	Valine/unknown	α-CH	0.9 (0.13)	0.5 (0.08)
3.61	d/m	Threonine/ unknown	α-CH	1.01 (0.15)	0.62 (0.11)
3.63		Unknown		1.04 (0.25)	0.56 (0.05)
3.65	m	SN-GPC	NCH_2	0.99 (0.28)	0.55 (0.05)
3.67	m	SN-GPC	NCH_2	0.94 (0.18)	0.51 (0.06)
3.79	dd	Glucose	Half CH_2-C6 of α-Glucose	1.04 (0.31)	0.69 (0.14)
3.87	m	Glucose	Half CH_2-C6 of α-Glucose	1.01 (0.18)	0.6 (0.1)
3.95	dd/s	Glucose/Creatine	Half CH_2-C6 of β-glucose	0.96 (0.23)	0.6 (0.1)
3.97	m	Phenylalanine	α-CH	0.99 (0.03)	0.59 (0.09)
3.99	m	Phenylalanine/ Lipids	α-CH/CH_2OCOR	0.98 (0.08)	0.55 (0.07)
4.29	m	Lipids	OCH_2	1.06 (0.27)	0.51 (0.09)
4.31	m	Lipids	OCH_2	0.93 (0.17)	0.48 (0.09)
5.25	m	Unsaturated Lipids	CH=$CHCH_2CH$=CH	0.99 (0.21)	0.51 (0.05)
5.27	m	Unsaturated Lipids	=$CHCH_2CH_2$	1.02 (0.17)	0.5 (0.11)
5.29	m	Unsaturated Lipids	CH=$CHCH_2CH$=CH	1.01 (0.16)	0.48 (0.1)
5.31	m	Unsaturated Lipids	=$CHCH_2CH_2$	1 (0.19)	0.49 (0.14)

Table S2. Comparison of profiled metabolite concentrations using Chenomx Profiler.

Metabolite	Concentration (mM)					
	Sham			Trauma		
	Before Mean (SD)	After Mean (SD)	FC Mean (SD)	Before Mean (SD)	After Mean (SD)	FC Mean (SD)
3-Hydroxybutyrate	0.067 (0.038)	0.034 (0.013)	0.62 (0.342)	0.028 (0.018)	0.034 (0.011)	9.596 (19.16)
3-Hydroxyisovalerate	0.013 (0.001)	0.009 (0.005)	0.676 (0.300)	0.013 (0.002)	0.007 (0.005)	0.506 (0.313)
Acetate	0.125 (0.062)	0.108 (0.056)	0.883 (0.205)	0.175 (0.058)	0.186 (0.034)	1.146 (0.38)
Acetone	0.069 (0.066)	0.061 (0.054)	1.106 (0.362)	0.07 (0.051)	0.046 (0.037)	0.618 (0.215)
Alanine	0.424 (0.048)	0.453 (0.098)	1.069 (0.221)	0.461 (0.094)	0.439 (0.073)	0.989 (0.283)
Arginine	0.261 (0.038)	0.253 (0.052)	0.988 (0.299)	0.239 (0.037)	0.154 (0.02)	0.661 (0.153)*
Betaine	0.112 (0.028)	0.096 (0.042)	0.827 (0.194)	0.13 (0.073)	0.08 (0.04)	0.61 (0.181)
Choline	0 (0)	0.001 (0.002)	2.25 (2.50)	0 (0)	0.009 (0.002)	12.213 (2.562)*
Citrate	0.14 (0.029)	0.13 (0.022)	0.938 (0.076)	0.166 (0.022)	0.126 (0.033)	0.754 (0.131)
Creatine	0.266 (0.149)	0.257 (0.137)	1.078 (0.447)	0.168 (0.079)	0.136 (0.091)	0.75 (0.248)
Creatinine	0.136 (0.028)	0.125 (0.041)	0.904 (0.147)	0.106 (0.008)	0.101 (0.018)	0.96 (0.181)
Formate	0.009 (0.011)	0.016 (0.005)	9.75 (10.252)	0.005 (0.007)	0.014 (0.007)	10.286 (11.892)
Glucose	2.963 (0.622)	2.781 (0.698)	0.981 (0.34)	3.9 (0.989)	3.886 (0.93)	1.036 (0.332)
Glutamate	0.2 (0.038)	0.169 (0.053)	0.853 (0.257)	0.184 (0.047)	0.162 (0.032)	0.899 (0.151)
Glutamine	0.33 (0.026)	0.297 (0.012)	0.907 (0.107)	0.38 (0.042)	0.285 (0.046)	0.756 (0.155)
Glycine	1.12 (0.227)	1.041 (0.348)	0.919 (0.149)	1.011 (0.142)	0.747 (0.172)	0.74 (0.153)
Hypoxanthine	0.004 (0.009)	0 (0)	0.761 (0.478)	0 (0)	0.01 (0.011)	14.027 (14.352)
Isoleucine	0.127 (0.032)	0.13 (0.027)	1.059 (0.287)	0.09 (0.019)	0.09 (0.018)	1.022 (0.24)
Lactate	1.493 (0.231)	2.073 (1.418)	1.472 (1.202)	1.446 (0.397)	2.328 (1.137)	1.758 (1.022)
Leucine	0.136 (0.027)	0.15 (0.015)	1.121 (0.117)	0.141 (0.049)	0.125 (0.025)	0.958 (0.348)
Lysine	0.085 (0.029)	0.081 (0.03)	1.026 (0.358)	0.065 (0.038)	0.09 (0.029)	2.726 (3.254)
Methionine	0.046 (0.015)	0.04 (0.006)	0.913 (0.217)	0.038 (0.009)	0.032 (0.009)	0.864 (0.28)
N-Nitrosodimethyl-amine	0.034 (0.016)	0.028 (0.017)	0.79 (0.235)	0.027 (0.006)	0.019 (0.008)	0.706 (0.164)
Phenylalanine	0.057 (0.01)	0.055 (0.013)	0.979 (0.185)	0.04 (0.011)	0.058 (0.02)	1.505 (0.538)
Proline	0.226 (0.029)	0.218 (0.066)	0.996 (0.400)	0.168 (0.076)	0.139 (0.029)	1.358 (1.507)
Pyruvate	0.101 (0.013)	0.129 (0.077)	1.337 (0.983)	0.122 (0.026)	0.113 (0.026)	0.961 (0.285)
Succinate	0.004 (0.003)	0.006 (0.001)	1.932 (1.125)	0.005 (0.003)	0.017 (0.02)	2.937 (2.02)
Threonine	0.211 (0.017)	0.164 (0.029)	0.776 (0.121)	0.169 (0.059)	0.109 (0.021)	0.683 (0.18)
Tyrosine	0.063 (0.009)	0.062 (0.006)	0.991 (0.146)	0.055 (0.003)	0.056 (0.01)	1.027 (0.18)
Urea	0.831 (0.629)	0.771 (0.656)	1.149 (0.62)	0.226 (0.224)	0.215 (0.481)	0.816 (0.863)
Valine	0.267 (0.06)	0.259 (0.029)	1.007 (0.234)	0.207 (0.041)	0.179 (0.027)	0.885 (0.201)

* Significant based on Wilcoxon-Mann-Whitney significance test of fold change values ($p < 0.05$).

Table S3. Fold change values of LC-MS metabolites identified to be significantly changed after trauma.

Metabolite ID	MZ/RT	Mode	Other modes	FC Sham Mean (SD)	FC Trauma[a] Mean (SD)
Citrulline	176.1029/23.1	H(+)		1.07 (0.17)	1.4 (0.3)*
L-methionine	133.0316/14.92	H(+)		0.94 (0.06)	1.34 (0.39)**
4-Methylene-L-glutamine	159.0768/23.1	H(+)		1.06 (0.1)	1.33 (0.32)**
Cysteine-Homocysteine disulfide	253.0315/23.94	H(-)		0.95 (0.18)	2.55 (0.93)**
L-Cysteinylglycine disulfide	298.053/24.42	H(+)		0.93 (0.19)	1.98 (0.95)**
L-Cystine	241.0314/24.1	H(+)	R(+)	0.95 (0.11)	1.6 (0.7)**
N1,N12-Diacetylspermine	287.2446/25.22	H(+)		1.1 (0.35)	2.22 (0.86)**
N1-acetylspermidine	188.1763/25.51	H(+)		1.09 (0.27)	2.34 (1.23)**
Pantothenic Acid	218.103/1.64	R(-)		0.87 (0.07)	1.37 (0.27)**
Phenylethylamine	105.034/2.73	H(+)		0.72 (0.2)	1.35 (0.42)**

S-(Hydroxymethyl)glutathione	336.0704/19.16	H(-)	R(-)	0.79 (0.29)	1.58 (0.32)**
S-Adenosylmethionine	399.1448/24.54	H(+)		0.98 (0.18)	1.99 (0.71)**
2,4-Diamino-butyric acid	117.0199/1.01	R(-)		0.79 (0.2)	2.7 (1.65)**
2,6-Diamino-heptanedioic acid	189.0404/0.96	R(-)		0.93 (0.17)	1.67 (0.71)**
4-(2-Aminophenyl)-2,4-dioxobutanoic acid	206.0457/4.62	R(-)	R(+), H(+)	1.03 (0.25)	2.13 (0.71)**
Glutarylcarnitine	276.144/16.1	H(+)		0.87 (0.8)	6.6 (4.27)**
3-indolecarboxylic acid glucuronide	338.087/19	H(+)		0.8 (0.37)	2.33 (1.21)**
4'-Methyl-(-)-epigallocatechin 7-glucuronide	495.1146/6.24	H(-)		0.84 (0.25)	2.65 (1.71)**
p-Cresol Glucuronide	283.0821/5.93	R(-)	H(-), R(+)	0.86 (0.23)	2.22 (0.71)**
Phenethylamine glucoronide, [M+FA-H]-	342.1186/1.07	R(-)		1.16 (0.14)	3.59 (1.93)*
N-butyrylglycine	144.0663/2.91	H(-)		0.69 (0.22)	2.48 (3.09)**
Phenylacetylgycine	192.0668/5.47	R(-)	H(+)	0.83 (0.15)	2.09 (0.64)**
Hippuric Acid (Benzoylglycine)	178.0513/4.29	R(-)	R(+), H(+)	0.75 (0.11)	1.78 (0.44)**
Adrenic acid	331.2628/14.04	R(-)		1.24 (0.33)	0.6 (0.23)**
Eicosadienoic acid	307.2626/14.44	R(-)		1.21 (0.56)	0.45 (0.25)**
LPC(17:0)	510.3554/11.18	R(+)		1.02 (0.24)	0.61 (0.11)**
LPC(20:3)	546.3555/10.46	R(+)		1.06 (0.14)	0.49 (0.19)**
LPC(22:4)	572.3714/10.93	R(+)		1.09 (0.11)	0.46 (0.13)**
LPC(22:5)	570.3558/10.2	R(+)	R(-)	1.09 (0.15)	0.44 (0.14)**
LPC(O-18:1)	508.3754/15.44	H(+)		1.01 (0.3)	0.44 (0.12)**
LPC(P-16:0)	480.344/14.86	H(+)		1.01 (0.09)	0.44 (0.11)**
PA(15:1)	375.1824/1.24	H(-)		0.95 (0.11)	0.53 (0.12)**
PA(29:2)	603.2906/12.67	H(+)		1.06 (0.19)	0.51 (0.28)*
PA(18:0), [M+Cl]-	473.1437/6.69	R(-)		0.91 (0.3)	1.9 (0.46)**
PA(18:1), [M+Na]+	459.1281/11.73	H(+)		0.99 (0.43)	2.73 (1.22)**
PA(18:4)	431.096/13.22	H(+)		0.67 (0.33)	2.51 (2.02)**
PA(19:3)	445.3291/1.21	H(-)		1.19 (0.23)	0.57 (0.12)**
PA(20:4)	459.2496/11.45	H(+)		1.18 (0.57)	0.62 (0.17)*
Lyso PAF C-16, [M+Cl]-	516.3184/15.76	H(-)		0.94 (0.07)	0.57 (0.2)**
Choline	104.108/13.5	H(+)		0.77 (0.17)	1.41 (0.39)**
PC(14:0)	468.308/15.42	H(+)		1 (0.09)	0.51 (0.12)**
PC(15:0)	480.3082/10.42	R(-)	H(+)	1.19 (0.26)	0.65 (0.18)**
PC(16:0)	496.3407/15.25	H(+)	R(+)	0.96 (0.08)	0.58 (0.08)**
PC(36:5)	780.5517/13.2	H(+)		1.35 (0.59)	0.61 (0.27)*
PC(21:0)	608.3173/10.42	R(-)		1.08 (0.29)	0.59 (0.18)**
PC(16:1)	494.3232/15.29	H(+)	R(+)	0.99 (0.08)	0.57 (0.1)**
PC(17:0)	510.3541/15.17	H(+)		0.94 (0.06)	0.61 (0.11)**
PC(26:0)	650.3458/14.92	H(+)		1.12 (0.18)	0.56 (0.14)**
PC(17:1)	508.3381/15.19	H(+)	R(-)	1.14 (0.35)	0.72 (0.17)**
PC(18:0)	524.3723/12.06	R(+)		1.1 (0.26)	0.55 (0.12)**
PC(20:0)	564.3302/9.92	R(-)		1.02 (0.21)	0.5 (0.22)**
PC(32:1)	590.3451/10.45	R(-)		1.11 (0.12)	0.52 (0.22)**
PC(18:1)	522.3547/15.11	H(+)	R(+), R(-)	0.99 (0.05)	0.6 (0.1)**
PC(18:2)	520.3398/15.19	H(+)	R(+)	0.96 (0.05)	0.57 (0.1)**
PC(18:3)	518.3229/15.25	H(+)		1 (0.08)	0.59 (0.11)**
PC(20:1)	550.3841/14.98	H(+)		0.96 (0.16)	0.49 (0.14)**
PC(20:2)	548.3686/15.04	H(+)	R(+)	0.94 (0.16)	0.54 (0.15)**
PC(20:4)	544.3394/15	H(+)	R(+)	1 (0.03)	0.55 (0.13)**
PC(20:5)	542.3221/15.09	H(+)	R(+)	1.01 (0.11)	0.59 (0.13)**
PC(22:4), [M+FA-H]-	616.3612/10.95	R(-)		0.99 (0.19)	0.41 (0.14)**
PC(22:6)	568.3386/14.95	H(+)	R(+), R(-)	1.06 (0.05)	0.46 (0.13)**
PC(O-15:0/O-1:0)	482.3605/11.15	R(+)		1.05 (0.21)	0.62 (0.09)**
PC(O-16:0/0:0)	482.3602/15.58	H(+)		1.01 (0.17)	0.47 (0.09)**

PC(O-18:0/20:4)	796.6183/13.27	H(+)		1.26 (0.41)	0.56 (0.4)*
SN-Glycero-3-phosphocholine	258.1111/23.56	H(+)		0.93 (0.19)	0.4 (0.14)**
PE(18:2)	478.2917/12.63	H(+)		1.17 (0.23)	0.64 (0.16)**
PE(20:4)	502.2919/12.37	H(+)	R(-)	1.38 (0.16)	0.67 (0.11)**
PE(22:4)	528.3087/9.91	R(-)		1.08 (0.18)	0.59 (0.2)**
PE(22:6)	526.2919/12.35	H(+)		1.28 (0.16)	0.81 (0.23)**
PE(O-18:1)	466.3281/12.17	H(+)		1.05 (0.28)	0.62 (0.15)**
PE(P-16:0)	438.2968/12.26	H(+)	R(+)	1.06 (0.21)	0.64 (0.14)**
PG(20:2)	537.1672/11.2	H(+)		1.46 (0.91)	4.73 (3.93)*
PI(17:1)	585.2701/1.2	H(+)		0.83 (0.21)	0.56 (0.12)*
PI(18:0)	599.3195/10.1	R(-)		0.98 (0.22)	0.56 (0.23)*
PI(20:4)	619.2847/12.81	H(-)		0.87 (0.2)	0.38 (0.16)**
PI(P-18:0)	585.2702/15.11	R(+)		0.93 (0.12)	0.49 (0.1)**
PS(38:6)	806.502/10.42	R(-)		1.27 (0.28)	0.61 (0.3)**
PS(18:2)	520.264/13.78	H(-)		1.23 (0.27)	0.62 (0.27)**
PS(19:0)	538.3138/9.53	R(-)		1.01 (0.04)	0.63 (0.19)**
PS(22:6)	568.3612/12.08	R(-)		1.08 (0.25)	0.56 (0.17)**
PS(20:0)	566.3459/10.78	R(-)		1 (0.16)	0.51 (0.19)**
Cer(d18:0/16:0)	540.3653/15.64	H(+)		1.28 (0.41)	0.56 (0.17)**
CerP(d18:1/14:0)	588.3301/9.9	R(-)		1.04 (0.16)	0.53 (0.26)**
NeuAcα2-3Galβ-Cer(d18:1/16:0)	991.6709/15.23	H(+)		1.14 (0.47)	0.25 (0.08)**
C16 Sphingosine-1-phosphate	350.1488/12.72	H(-)		0.66 (0.16)	0.31 (0.11)**
Psychosine Sulfate	540.33/10.42	R(-)		1.06 (0.21)	0.55 (0.16)**
SM(d16:1/18:1)	701.5579/14.48	H(+)		1.37 (0.84)	0.66 (0.23)*
SM(d18:1/14:0)	675.5417/14.55	H(+)		1.41 (0.93)	0.73 (0.33)*
1-Methylguanosine	298.114/1.24	R(+)	H(+)	1.13 (0.09)	1.54 (0.38)**
1-methylnicotinamide	137.071/14.26	H(+)		0.93 (0.06)	3.89 (5.68)**
1-methyluric Acid	181.0359/10.41	H(-)		0.99 (0.33)	2.25 (0.67)**
3-Methylguanine	166.0717/9.63	H(+)		0.94 (0.18)	1.8 (0.64)**
3'-O-Methyladenosine	282.1196/17.53	H(+)		0.99 (0.23)	1.46 (0.37)**
3'-O-Methylguanosine	298.114/11.76	H(+)		0.97 (0.18)	1.66 (0.61)**
7-Methylguanine	166.0719/7.73	H(+)		0.87 (0.21)	1.55 (0.59)**
N2-Methylguanine	166.072/11.76	H(+)		0.93 (0.13)	1.83 (0.82)**
Ascorbic Acid	175.0249/0.79	R(-)		1.01 (0.47)	4.72 (3.46)**
7-alpha-Hydroxy-3-oxo-4-cholestenoate	431.3158/10.35	R(+)		0.96 (0.09)	0.64 (0.18)**
9,12,15-Octadecatrien-1-ol	265.2523/14.18	R(+)		1.3 (0.34)	0.71 (0.22)*
Galactosamine-1-phosphate	260.0742/23.31	H(+)		1.12 (0.21)	2.37 (0.86)*
Isobuteine	206.0456/4.8	H(-)		1.03 (0.16)	1.8 (0.56)**
N1-(5-Phospho-a-D-ribosyl)-5,6-dimethylbenzimidazole	357.0818/1.83	R(-)		0.98 (0.31)	1.94 (0.49)**
Taurochenodeoxycholic acid 7-sulfate	580.4305/14.83	H(+)		1.25 (0.35)	0.52 (0.19)**
Aspartyl-aspartate	249.0753/5.94	R(+)		0.93 (0.12)	1.91 (0.69)**
Glutaminyl-Serine, [M+H-H2O]+	216.0974/17.09	H(+)		1.37 (1.15)	0.29 (0.26)*
Hydroxyprolyl-glutamine	258.108/23.73	H(-)		1.35 (0.68)	0.5 (0.15)**
Methionyl-Glutamate, [M+HAc-H]-	336.1388/23.43	H(-)		0.87 (0.31)	3.23 (1.73)**
Phenylalanine-Tryptophan	352.1644/12.64	H(+)		0.88 (0.23)	0.46 (0.13)**
Phenylalanyl-Glutamine	292.0808/12.23	H(-)		0.97 (0.18)	1.98 (0.79)**
Serinyl-Methionine	235.082/1.34	R(-)		1.67 (0.38)	3.75 (1.26)**
6,8-Dihydroxypurine	153.0402/12.22	H(+)		1.01 (0.15)	2.94 (1.18)**
Adenosine	250.0928/1.94	H(+)		0.87 (0.32)	2.71 (2.1)*
Deoxyguanosine	266.0878/12.32	H(-)		1.43 (0.67)	6.43 (3.29)**
Guanosine	282.0829/14.25	H(-)	R(+), R(-)	1.22 (0.5)	3.73 (2.09)**
Hypoxanthine	137.0462/11.17	H(-)	H(+)	1 (0.28)	3.08 (1.99)**
Inosine	269.0876/11.18	H(+)	R(+), R(-)	1.38 (0.62)	3.77 (2.24)**

Succinoadenosine	382.0993/1.79	R(-)		1.03 (0.15)	2.09 (0.61)**
Uric Acid	169.0348/14.69	H(+)	R(-)	0.72 (0.32)	5.43 (4.78)**
Xanthosine	285.0818/12.17	H(+)	R(-)	1 (0.35)	2.65 (0.95)**
Cytosine	112.0505/9.76	H(+)		0.61 (0.16)	1.66 (0.52)**
5-hydroxymethyldeoxycytidylic acid	320.0615/3.36	H(+)		0.77 (0.22)	2.87 (2.2)*
Cytidine, [M+H-H2O]+	226.0817/9.78	H(+)		0.94 (0.14)	1.72 (0.49)**
Cytidine Monophosphate	322.2006/1.33	H(-)		0.97 (0.16)	0.54 (0.16)**
Thymidine	241.0824/1.38	R(-)		1 (0.17)	1.82 (0.43)**
Thymine	127.05/1.77	H(+)		1.1 (0.21)	1.64 (0.34)*
Uridine	243.0618/0.92	R(-)		0.81 (0.19)	2.07 (0.73)**

[a] Significant based on Wilcoxon-Mann-Whitney significance test of fold change values for Sham vs Trauma: *$p < 0.05$ **$p < 0.01$.

Table S4. Top metabolic pathways affected after the trauma injury.

	Total Cmpd	Hits	Raw p	-log(p)	Holm adjust	FDR	Impact
Glycerophospholipid metabolism	36	8	5.274E-07	6.278	1.002E-05	5.274E-06	0.137
Purine metabolism	65	7	0.005	2.300	0.033	0.007	0.025
Sphingolipid metabolism	21	5	1.565E-06	5.806	2.816E-05	1.043E-05	0.294
Pyrimidine metabolism	39	4	0.001	3.267	0.006	0.001	0.117
Cysteine and methionine metabolism	33	3	0.033	1.484	0.090	0.035	0.157
Arginine biosynthesis	14	2	7.473E-04	3.127	0.008	0.001	0.305
Phenylalanine metabolism	10	2	4.405E-04	3.356	0.006	0.001	0.238
Arginine and proline metabolism	38	2	0.002	2.728	0.017	0.003	0.058
Primary bile acid biosynthesis	46	2	7.422E-05	4.130	0.001	0.000	0.051
Ether lipid metabolism	20	2	4.683E-08	7.330	9.365E-07	9.37E-07	0.000
Aminoacyl-tRNA biosynthesis	48	2	0.001	2.960	0.011	0.002	0.000

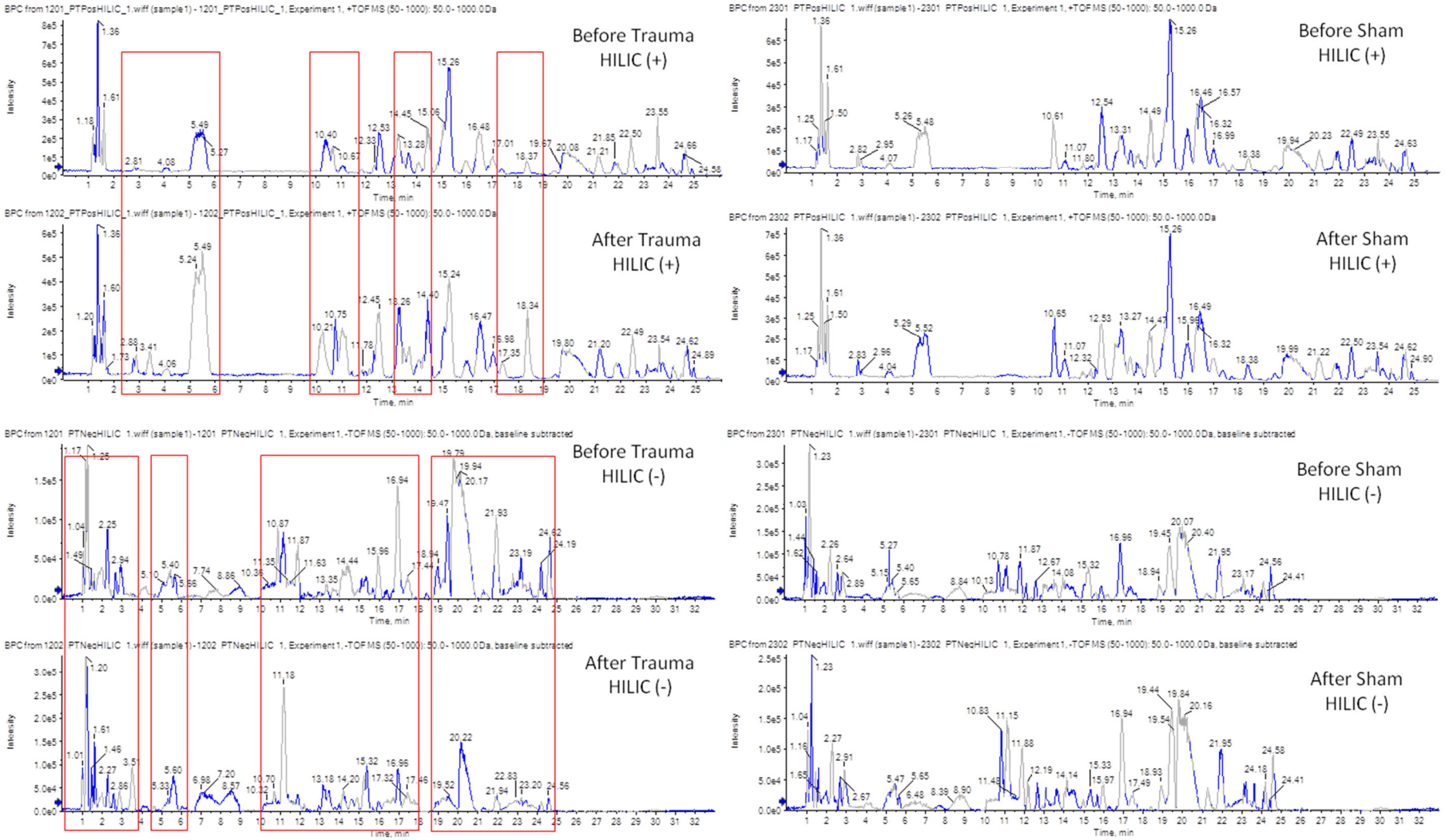

Figure S1. Comparison of base peak chromatograms of the HILIC LC-MS analyses for the sham and trauma samples.

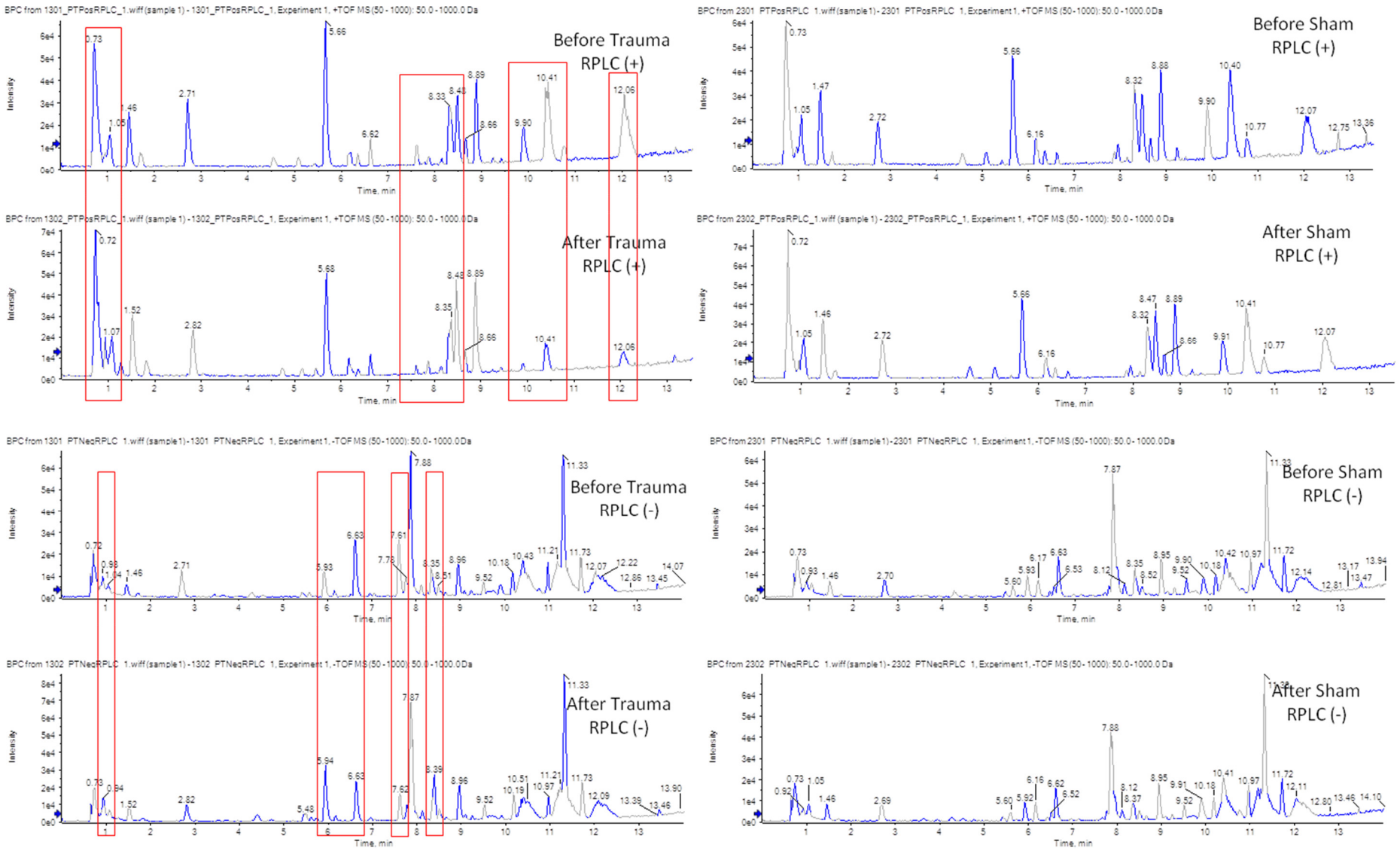

Figure S2. Comparison of BPCs of the RP LC-MS analyses for the sham and trauma samples.

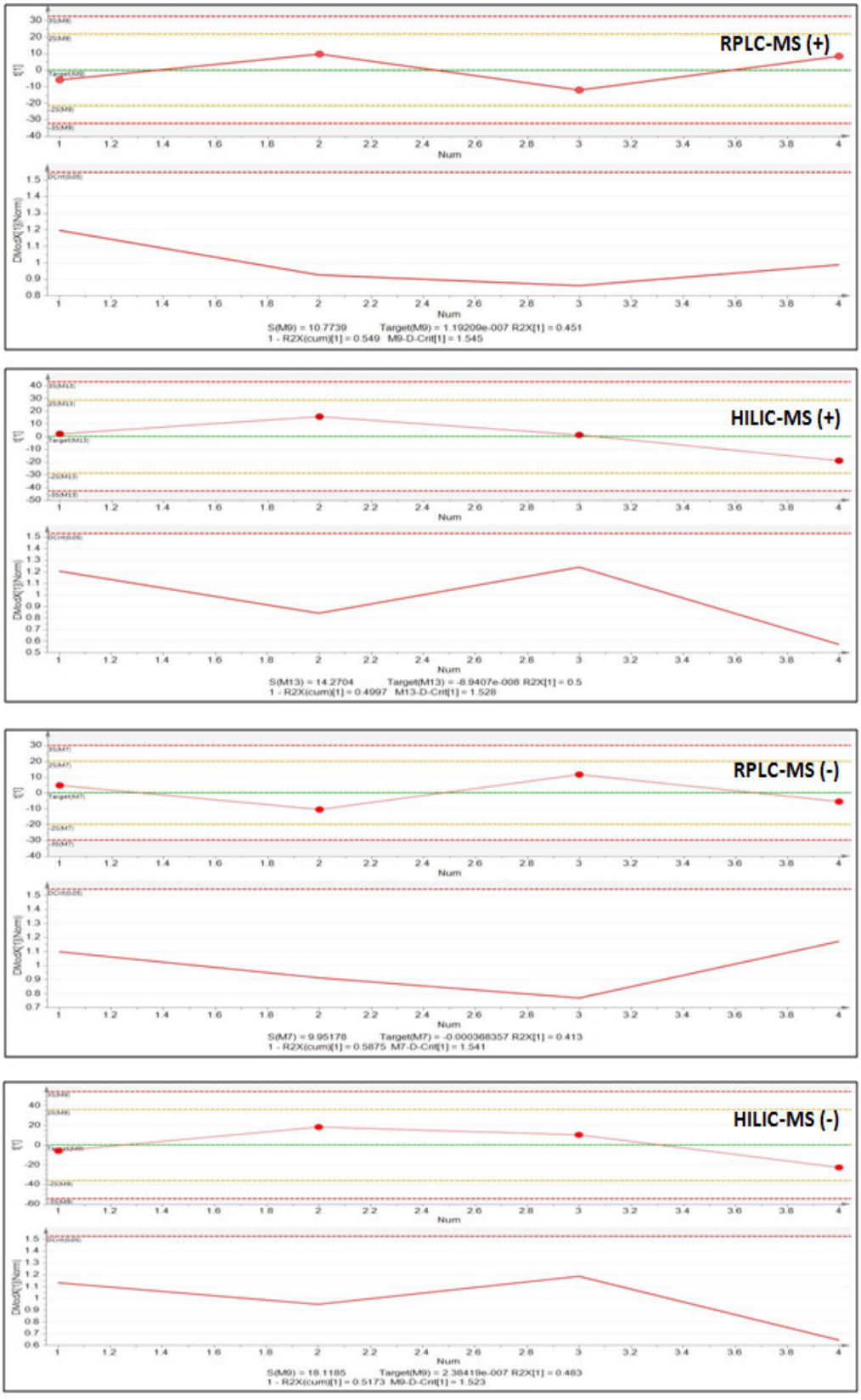

Figure S3. Shewhart control charts of the LC-MS pooled QC samples.