Supplementary Data

Supplementary Table S1. List of Metabolites Identified and Characterized by Liquid Chromatography Mass Spectrometry

No.	*Metabolite*	*No*	*Metabolite*
1	(R)-3-Hydroxydecanoic acid	96	Isovalerylglycine
2	(R)-lipoic acid	97	Itaconic acid
3	1-Methyladenosine	98	Kynurenic acid
4	1-Methylhistidine	99	L-Acetylcarnitine
5	1-Methylnicotinamide	100	L-Alanine
6	2'-Deoxyguanosine 5'-monophosphate	101	L-Arginine
7	2-Furoic acid	102	L-Asparagine
8	2-Hydroxycaproic acid	103	L-Aspartic acid
9	2-Hydroxyvaleric acid	104	L-Carnitine
10	2-Isopropyl-3-oxosuccinate	105	L-Cystathionine
11	2-Isopropylmalic acid	106	L-Dihydroorotic acid
12	2-Ketobutyric acid	107	L-Glutamic acid
13	2-Ketohexanoic acid	108	L-Glutamine
14	2-Pyrocatechuic acid	109	L-Histidine
15	3-hydroxyhexadecanoic acid	110	L-Histidinol
16	3-Hydroxymethylglutaric acid	111	L-Isoleucine
17	4-Acetamidobutanoic acid	112	L-Kynurenine
18	4-Hydroxybenzaldehyde	113	L-Lactic acid
19	4-Hydroxybutyric acid	114	L-Leucine
20	4-Pyridoxic acid	115	L-Lysine
21	5-Methoxytryptophan	116	L-Methionine
22	5-Methyltetrahydrofolic acid	117	L-Phenylalanine
23	5'-Methylthioadenosine	118	L-Proline
24	Acetylcholine	119	L-Serine
25	Acetylcysteine	120	L-Threonine
26	Acetylphosphate	121	L-Tryptophan
27	Adenine	122	L-Tyrosine
28	Adenosine	123	L-Valine
29	Adenosine monophosphate	124	Maleic acid
30	ADP	125	Malic acid
31	ADP-glucose	126	Mannitol
32	Allantoin	127	Methionine sulfoxide
33	Aminoadipic acid	128	Methylacetoacetic acid
34	Arecoline	129	Methylimidazoleacetic acid
35	Argininosuccinic acid	130	N6-Acetyl-L-lysine
36	Ascorbic acid	131	N-Acetylasparagine
37	Asymmetric dimethylarginine	132	N-Acetylaspartylglutamic acid
38	Beta-D-Glucopyranuronic acid	133	N-Acetyl-D-glucosamine
39	Betaine	134	N-Acetyl-glucosamine 1-phosphate
40	Betaine aldehyde	135	N-Acetylglutamic acid
41	Caprylic acid	136	N-Acetylglutamine
42	Carnosine	137	N-Acetyl-L-alanine
43	CDP-Ethanolamine	138	N-Acetyl-L-aspartic acid
44	Choline	139	N-Acetyl-L-methionine
45	Citicoline	140	N-Acetylornithine
46	Citric acid	141	N-Acetylputrescine
47	Citrulline	142	NAD
48	Creatine	143	NADP
49	Creatinine	144	N-Formyl-L-methionine
50	Cytidine	145	Niacinamide
51	Cytidine monophosphate	146	Nicotinic acid
52	Cytosine	147	Ornithine
53	D-2-Hydroxyglutaric acid	148	Orotic acid
54	D-Arabitol	149	Orotidine

(*continued*)

SUPPLEMENTARY TABLE S1. (CONTINUED)

No.	*Metabolite*	*No*	*Metabolite*
55	Deoxyadenosine	150	Oxalacetic acid
56	Deoxyribose 5-phosphate	151	Oxidized glutathione (GSSG)
57	Deoxyuridine	152	Oxoglutaric acid
58	D-Fructose	153	Pantothenic acid
59	D-Glucose	154	Phenylacetylglycine
60	Dihydroxyacetone phosphate	155	Phenyllactic acid
61	Dimethylglycine	156	Phenylpyruvic acid
62	DL-2-Aminooctanoic acid	157	Phosphoenolpyruvic acid
63	D-Ribose	158	Phosphorylcholine
64	D-Ribose 5-phosphate	159	Pipecolic acid
65	D-Sedoheptulose 7-phosphate	160	Proline betaine
66	Ecgonine	161	Propionylcarnitine
67	Fructose 6-phosphate	162	Putrescine
68	GDP-glucose	163	Pyridoxamine
69	Gluconic acid	164	Pyridoxine
70	Gluconolactone	165	Pyroglutamic acid
71	Glucosamine 6-phosphate	166	Pyruvic acid
72	Glucose 1-phosphate	167	Quinolinic acid
73	Glucose 6-phosphate	168	S-Adenosylhomocysteine
74	Glutathione reduced (GSH)	169	S-Adenosylmethionine
75	Glycerol 3-phosphate	170	Salicylic acid
76	Glycerophosphocholine	171	Spermidine
77	Glycine	172	Succinic acid
78	Glycolic acid	173	Taurine
79	Glyoxylic acid	174	Thiamine
80	Guanidoacetic acid	175	Thiamine monophosphate
81	Guanine	176	Threonic acid
82	Guanosine	177	Thymidine
83	Guanosine diphosphate	178	trans-Aconitic acid
84	Hexanoylcarnitine	179	Uracil
85	Hippuric acid	180	Ureidosuccinic acid
86	Hydrocinnamic acid	181	Uric acid
87	Hypotaurine	182	Uridine
88	Hypoxanthine	183	Uridine 5'-monophosphate
89	Imidazoleacetic acid	184	Uridine diphosphate glucuronic acid
90	Imidazolelactic acid	185	Uridine diphosphategalactose
91	Indole-3-carboxylic acid	186	Uridine diphosphate-N-acetylglucosamine
92	Indolelactic acid	187	Urocanic acid
93	Inosine	188	Vanillin
94	Inosinic acid	189	Xanthine
95	Insitol	190	Xanthosine

Metabolites significantly altered in the ipsilateral hemisphere after traumatic brain injury (untreated) when compared with sham are highlighted. Metabolites decreased (light gray) and increased (dark gray).