

## Supplementary Material to:

### Metabolic Phenotypes of Hypoxic-Ischemic Encephalopathy

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**Supplementary Table 1.** Annotation of altered metabolites. Note: blue stands for detected, but not altered; red stands for altered; IDs of annotated metabolites marked with a star have been verified with MS/MS data.

Pathway	KEGG	Name	Mol Form	T0	T24	T48	T72	Adduct	m/z	
Steroid hormone biosynthesis	C00735	Cortisol	C21H30O5	Blue	Red	Red	Red	[M+H] <sup>+</sup>	363.2166	
	C01780	Aldosterone	C21H28O5	Blue	Red	Red	Red	[M+H] <sup>+</sup>	361.2010	
	C01124	18-Hydroxycorticosterone	C21H30O5	Blue	Red	Red	Red	[M+H] <sup>+</sup>	363.2166	
	C00187	Cholesterol	C27H46O	Blue	Blue	Red	Blue	[M+HCOONa] <sup>+</sup>	455.3496	
	C01953	Pregnenolone	C21H32O2	Red	Red	Red	Red	[M+H] <sup>+</sup>	317.2475	
	C01227	Dehydroepiandrosterone	C19H28O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	311.1982	
	C04295	Androstenediol	C19H30O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	313.2138	
	C03205	11-Deoxycorticosterone	C21H30O3	Red	Red	Red	Red	[M+H] <sup>+</sup>	331.2268	
	C02140	Corticosterone	C21H30O4	Red	Red	Red	Red	[M+H] <sup>+</sup>	347.2217	
	C00410	Progesterone	C21H30O2	Blue	Red	Red	Red	[M+H] <sup>+</sup>	315.2319	
	C03681	5alpha-Pregnane-3,20-dione	C21H32O2	Red	Red	Red	Red	[M+H] <sup>+</sup>	317.2475	
	C01176	17alpha-Hydroxyprogesterone	C21H30O3	Red	Red	Red	Red	[M+H] <sup>+</sup>	331.2268	
	C00762	Cortisone	C21H28O5	Blue	Red	Red	Red	[M+H] <sup>+</sup>	361.2010	
	C00535	Testosterone	C19H28O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	311.1982	
	C00280	Androstenedione*	C19H26O2	Blue	Blue	Blue	Red	[M+H] <sup>+</sup>	287.2006	
	C03772	5beta-Androstane-3,17-dione	C19H28O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	311.1982	
	C04373	Etiocholanolone	C19H30O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	313.2138	
	C00674	5alpha-Androstane-3,17-dione	C19H28O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	311.1982	
	C00523	Androsterone	C19H30O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	313.2138	
	C00468	Estrone	C18H22O2	Blue	Red	Red	Red	[M+H] <sup>+</sup>	271.1693	
	C03917	Dihydrotestosterone	C19H30O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	313.2138	
	C02538	Estrone 3-sulfate	C18H22O5S	Blue	Blue	Red	Red	[M-H2O+H] <sup>+</sup>	333.1155	
	C03747	11alpha-Hydroxyprogesterone	C21H30O3	Red	Red	Red	Red	[M+H] <sup>+</sup>	331.2268	
	C04042	20alpha-Hydroxy-4-pregnen-3-one	C21H32O2	Red	Red	Red	Red	[M+H] <sup>+</sup>	317.2475	
	C03852	Androstan-3alpha,17beta-diol	C19H32O2	Red	Red	Red	Red	[M+Na] <sup>+</sup>	315.2295	
	C03935	6beta-Hydroxy-17beta-estradiol	C18H24O3	Blue	Red	Red	Red	[M+K] <sup>+</sup>	327.1357	
	<b>Caffeine</b>	C01762	Xanthosine	C10H12N4O6	Red	Blue	Blue	Blue	[M+H] <sup>+</sup>	285.0830
	<b>metabolism</b>	C00385	Xanthine*	C5H4N4O2	Red	Blue	Blue	Blue	[M+H] <sup>+</sup>	153.0407
	<b>Selenoamino</b>	C00979	O-Acetyl-L-serine	C5H9NO4	Red	Blue	Blue	Blue	[M+H] <sup>+</sup>	148.0604
	<b>acid metabolism</b>	C00041	L-Alanine	C3H7NO2	Red	Blue	Blue	Blue	[M+H] <sup>+</sup>	90.0550

Phenylalanine metabolism	C03589	4-Hydroxy-2-oxopentanoate	C5H8O4					[M+H] <sup>+</sup>	133.0495	
	C00079	L-Phenylalanine	C9H11NO2					[M+H] <sup>+</sup>	166.0863	
	C00601	Phenylacetaldehyde	C8H8O					[M-H2O+H] <sup>+</sup>	103.0542	
	C00596	2-Hydroxy-2,4-pentadienoate	C5H6O3					[M+H2O+H] <sup>+</sup>	133.0495	
	C04044	3-(2,3-Dihydroxyphenyl)propanoate	C9H10O4					[M+H] <sup>+</sup>	183.0652	
	C00166	Phenylpyruvate	C9H8O3					[M+H] <sup>+</sup>	165.0546	
	C02265	D-Phenylalanine	C9H11NO2					[M+H] <sup>+</sup>	166.0863	
	C02505	2-Phenylacetamide	C8H9NO					[M+H] <sup>+</sup>	136.0757	
	C00423	trans-Cinnamate	C9H8O2					[M+H] <sup>+</sup>	149.0597	
	C01198	3-(2-Hydroxyphenyl)propanoate	C9H10O3					[M+H] <sup>+</sup>	167.0703	
	C00180	Benzoate	C7H6O2					[M+H] <sup>+</sup>	123.0441	
	C01586	Hippurate	C9H9NO3					[M+H] <sup>+</sup>	180.0655	
	C01722	trans-2-Hydroxycinnamate	C9H8O3					[M+H] <sup>+</sup>	165.0546	
	C00811	4-Coumarate	C9H8O3					[M+H] <sup>+</sup>	165.0546	
	C02137	alpha-Oxo-benzeneacetic acid	C8H6O3					[M+H] <sup>+</sup>	151.0390	
	C04148	Phenylacetylglutamine	C13H16N2O4					[M+H] <sup>+</sup>	265.1183	
	C00042	Succinate	C4H6O4					[M+H] <sup>+</sup>	119.0339	
	C00122	Fumarate	C4H4O4					[M-CO2+H] <sup>+</sup>	73.0284	
	C02763	2-Hydroxy-3-phenylpropenoate	C9H8O3					[M+H] <sup>+</sup>	165.0546	
	C03519	N-Acetyl-L-phenylalanine	C11H13NO3					[M+K] <sup>+</sup>	246.0527	
	C00156	4-Hydroxybenzoate	C7H6O3					[M+H] <sup>+</sup>	139.0390	
	C00642	4-Hydroxyphenylacetate	C8H8O3					[M+H] <sup>+</sup>	153.0546	
	C00805	Salicylate	C7H6O3					[M+H] <sup>+</sup>	139.0390	
	C00082	L-Tyrosine*	C9H11NO3					[M+H] <sup>+</sup>	182.0812	
	Arginine and proline metabolism	C01165	L-Glutamate 5-semialdehyde	C5H9NO3					[M+H] <sup>+</sup>	132.0655
		C04281	L-1-Pyrroline-3-hydroxy-5-carboxylate	C5H7NO3					[M+H] <sup>+</sup>	130.0499
		C00064	L-Glutamine	C5H10N2O3					[M+H] <sup>+</sup>	147.0764
		C00077	L-Ornithine	C5H12N2O2					[M+H] <sup>+</sup>	133.0972
		C00049	L-Aspartate	C4H7NO4					[M+H2O+H] <sup>+</sup>	152.0548
		C03406	L-Argininosuccinate	C10H18N4O6					[M+H] <sup>+</sup>	291.1299
C00025		L-Glutamate	C5H9NO4					[M+H] <sup>+</sup>	148.0604	
C00624		N-Acetyl-L-glutamate	C7H11NO5					[M+H] <sup>+</sup>	190.0710	
C04133		N-Acetyl-L-glutamate 5-phosphate	C7H12NO8P					[M-CO+H] <sup>+</sup>	242.0432	
C01250		N-Acetyl-L-glutamate 5-semialdehyde	C7H11NO4					[M+H] <sup>+</sup>	174.0761	

Arginine and proline metabolism

C00437	N-Acetylornithine	C7H14N2O3					[M+H] <sup>+</sup>	175.1077
C00148	L-Proline	C5H9NO2					[M+H] <sup>+</sup>	116.0706
C01877	4-Oxoproline	C5H7NO3					[M+H] <sup>+</sup>	130.0499
C00763	D-Proline	C5H9NO2					[M+H] <sup>+</sup>	116.0706
C03564	1-Pyrroline-2-carboxylate	C5H7NO2					[M+H] <sup>+</sup>	114.0550
C01157	Hydroxyproline	C5H9NO3					[M+H] <sup>+</sup>	132.0655
C01682	Nopaline	C11H20N4O6					[M-NH3+H] <sup>+</sup>	288.1185
C00300	Creatine	C4H9N3O2					[M+H] <sup>+</sup>	132.0768
C01043	N-Carbamoylsarcosine	C4H8N2O3					[M+NaCl] <sup>+</sup>	191.0179
C00791	Creatinine	C4H7N3O					[M+H] <sup>+</sup>	114.0662
C03771	5-Guanidino-2-oxopentanoate	C6H11N3O3					[M+H] <sup>+</sup>	174.0874
C02647	4-Guanidinobutanal	C5H11N3O					[M+Na] <sup>+</sup>	152.0787
C01035	4-Guanidinobutanoate	C5H11N3O2					[M+H] <sup>+</sup>	146.0924
C00334	4-Aminobutanoate	C4H9NO2					[M+H] <sup>+</sup>	104.0706
C03078	4-Guanidinobutanamide	C5H12N4O					[M+Na] <sup>+</sup>	167.0896
C00436	N-Carbamoylputrescine	C5H13N3O					[M+NaCl] <sup>+</sup>	190.0722
C03296	N2-Succinyl-L-arginine	C10H18N4O5					[M+NaCl] <sup>+</sup>	333.0910
C03415	N2-Succinyl-L-ornithine	C9H16N2O5					[M+H] <sup>+</sup>	233.1132
C03912	(S)-1-Pyrroline-5-carboxylate	C5H7NO2					[M+H] <sup>+</sup>	114.0550
C00555	4-Aminobutyraldehyde	C4H9NO					[M+H] <sup>+</sup>	88.0757
C01137	S-Adenosylmethioninamine	C14H23N6O3S					[M+H] <sup>+</sup>	356.1602
C00019	S-Adenosyl-L-methionine	C15H22N6O5S					[M+2H] <sup>+</sup>	200.0743
C02714	N-Acetylputrescine	C6H14N2O					[M+H] <sup>+</sup>	131.1179
C02946	4-Acetamidobutanoate	C6H11NO3					[M+H] <sup>+</sup>	146.0812
C03440	cis-4-Hydroxy-D-proline	C5H9NO3					[M+H] <sup>+</sup>	132.0653
C04282	1-Pyrroline-4-hydroxy-2-carboxylate	C5H7NO3					[M+H] <sup>+</sup>	130.0499
C00122	Fumarate	C4H4O4					[M-CO2+H] <sup>+</sup>	73.0286
C01110	5-Amino-2-oxopentanoic acid	C5H9NO3					[M+H] <sup>+</sup>	132.0655
C00431	5-Aminopentanoate	C5H11NO2					[M+H] <sup>+</sup>	118.0863
C04137	D-Octopine	C9H18N4O4					[M+H] <sup>+</sup>	247.1401
C00213	Sarcosine	C3H7NO2					[M+H] <sup>+</sup>	90.0550
C00884	Homocarnosine	C10H16N4O3					[M+H] <sup>+</sup>	241.1295
C03166	Phosphoguanidinoacetate	C3H8N3O5P					[M-CO+H] <sup>+</sup>	170.0330

Lysine biosynthesis	C00666	LL-2,6-Diaminoheptanedioate	C7H14N2O4					[M+H] <sup>+</sup>	191.1026	
	C00956	L-2-Aminoadipate	C6H11NO4					[M+H] <sup>+</sup>	162.0761	
	C00049	L-Aspartate	C4H7NO4					[M+H2O+H] <sup>+</sup>	152.0548	
	C03082	4-Phospho-L-aspartate	C4H8NO7P					[M-HCOOK+H] <sup>+</sup>	130.0499	
	C00263	L-Homoserine	C4H9NO3					[M+H] <sup>+</sup>	120.0655	
	C00441	L-Aspartate 4-semialdehyde	C4H7NO3					[M+H2O+H] <sup>+</sup>	136.0618	
	C03972	2,3,4,5-Tetrahydrodipicolinate	C7H9NO4					[M-H2O+H] <sup>+</sup>	190.0722	
	C03871	L-2-Amino-6-oxoheptanedioate	C7H11NO5					[M+H] <sup>+</sup>	190.0723	
	C04421	N-Succinyl-LL-2,6-diaminoheptanedioate	C11H18N2O7					[M+H2O+H] <sup>+</sup>	309.1265	
	C04390	N6-Acetyl-LL-2,6-diaminoheptanedioate	C9H16N2O5					[M+H] <sup>+</sup>	233.1132	
	C00680	meso-2,6-Diaminoheptanedioate	C7H14N2O4					[M+H] <sup>+</sup>	191.1029	
	C00449	N6-(L-1,3-Dicarboxypropyl)-L-lysine	C11H20N2O6					[M+H] <sup>+</sup>	277.1394	
	C01251	Homocitrate	C7H10O7					[M+H] <sup>+</sup>	207.0516	
	C00026	2-Oxoglutarate	C5H6O5					[M+HCOONa] <sup>+</sup>	215.0166	
	C00322	2-Oxadipate	C6H8O5					[M+H] <sup>+</sup>	161.0460	
	C03340	Dihydrodipicolinate	C7H7NO4					M-CO2+H[1+]	126.0549	
	C04462	N-Succinyl-2-L-amino-6-oxoheptanedioate	C11H15NO8					[M+H] <sup>+</sup>	290.0854	
	C04076	L-2-Aminoadipate 6-semialdehyde	C6H11NO3					[M+H] <sup>+</sup>	146.0812	
	C04002	cis-Homoaconitate	C7H8O6					[M+Na] <sup>+</sup>	211.0209	
	D-Glutamine and D-glutamate metabolism	C00819	D-Glutamine	C5H10N2O3					[M+H] <sup>+</sup>	147.0764
		C00217	D-Glutamate	C5H9NO4					[M+H] <sup>+</sup>	148.0604
		C01212	UDP-N-acetylmuramoyl-L-alanine	C23H36N4O20P2					M(S34)+H[1+]	753.1441
C00025		L-Glutamate	C5H9NO4					[M+H] <sup>+</sup>	148.0604	
C00064		L-Glutamine	C5H10N2O3					[M+H] <sup>+</sup>	147.0764	
C02237		5-Oxo-D-proline	C5H7NO3					[M+H] <sup>+</sup>	130.0499	
C00026		2-Oxoglutarate	C5H6O5					[M+HCOONa] <sup>+</sup>	215.0166	
Lysine degradation	C00739	D-Lysine	C6H14N2O2					[M+H] <sup>+</sup>	147.1128	
	C00047	L-Lysine	C6H14N2O2					[M+H] <sup>+</sup>	147.1128	
	C04092	Delta1-Piperideine-2-carboxylate	C6H9NO2					[M+H] <sup>+</sup>	128.0706	
	C00449	Saccharopine	C11H20N2O6					[M+H] <sup>+</sup>	277.1403	
	C01149	4-Trimethylammoniumbutanal	C7H16NO					[M+NaCl] <sup>+</sup>	189.0897	
	C03793	N6,N6,N6-Trimethyl-L-lysine	C9H20N2O2					[M+H] <sup>+</sup>	189.1598	
	C01144	(S)-3-Hydroxybutanoyl-CoA	C25H42N7O18P3S					[M+NaCl] <sup>+</sup>	912.1245	
	C00408	Pipecolic acid	C6H11NO2					[M+H] <sup>+</sup>	130.0863	

Lysine degradation	C02727	N6-Acetyl-L-lysine	C8H16N2O3					[M+H] <sup>+</sup>	189.1234	
	C04076	L-2-Aminoadipate 6-semialdehyde	C6H11NO3					[M+H] <sup>+</sup>	146.0812	
	C00956	L-2-Aminoadipate	C6H11NO4					[M+H] <sup>+</sup>	162.0761	
	C00322	2-Oxoadipate	C6H8O5					[M+H] <sup>+</sup>	161.0444	
	C00527	Glutaryl-CoA	C26H42N7O19P3S					M(C13)+2H[2 <sup>+</sup> ]	442.0844	
	C00489	Glutaric acid	C5H8O4					[M+H] <sup>+</sup>	133.0495	
	C03273	5-Oxopentanoate	C5H8O3					M+[HCOONa] <sup>+</sup>	185.0421	
	C00990	5-Aminopentanamide	C5H12N2O					[M-NH3+H] <sup>+</sup>	100.0758	
	C03087	5-Acetamidopentanoate	C7H13NO3					[M+H] <sup>+</sup>	160.0968	
	C01142	L-beta-Lysine	C6H14N2O2					[M+H] <sup>+</sup>	147.1128	
	C01186	(3S,5S)-3,5-Diaminohexanoate	C6H14N2O2					[M+H] <sup>+</sup>	147.1128	
	C03955	N6-Acetyl-N6-hydroxy-L-lysine	C8H16N2O4					[M+H] <sup>+</sup>	205.1183	
	C01028	N6-Hydroxy-L-lysine	C6H14N2O3					[M+H] <sup>+</sup>	163.1077	
	C04020	D-Lysopine	C9H18N2O4					[M+H] <sup>+</sup>	219.1339	
	C03239	6-Amino-2-oxohexanoate	C6H11NO3					[M+H] <sup>+</sup>	146.0812	
	C00487	Carnitine	C7H16NO3					[M+NaCl] <sup>+</sup>	221.0796	
	C03366	5-Phosphooy-L-lysine	C6H15N2O6P					[M+H2O+H] <sup>+</sup>	261.0872	
	C00450	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	C6H9NO2					[M+H] <sup>+</sup>	128.0706	
	C00431	5-Aminopentanoate	C5H11NO2					[M+H] <sup>+</sup>	118.0863	
	C03656	(S)-5-Amino-3-oxohexanoic acid	C6H11NO3					[M+H] <sup>+</sup>	146.0812	
	Nitrogen metabolism	C00079	L-Phenylalanine	C9H11NO2					[M+H] <sup>+</sup>	166.0863
		C00082	L-Tyrosine*	C9H11NO3					[M+H] <sup>+</sup>	182.0812
		C00078	L-Tryptophan*	C11H12N2O2					[M+H] <sup>+</sup>	205.0972
		C03618	L-threo-3-Methylaspartate	C5H9NO4					[M+H] <sup>+</sup>	148.0604
C00049		L-Aspartate	C4H7NO4					[M+H2O+H] <sup>+</sup>	152.0569	
C00152		L-Asparagine	C4H8N2O3					[M+NaCl] <sup>+</sup>	191.0179	
C00025		L-Glutamate	C5H9NO4					[M+H] <sup>+</sup>	148.0604	
C00064		L-Glutamine	C5H10N2O3					[M+H] <sup>+</sup>	147.0764	
C00108		Anthranilic acid	C7H7NO2					[M+H] <sup>+</sup>	138.0550	
C02291		L-Cystathionine	C7H14N2O4S					[M+Na] <sup>+</sup>	245.0589	
C00155		L-Homocysteine	C4H9NO2S					[M-NH3+H] <sup>+</sup>	119.0162	
C00542		Cystathionine	C7H14N2O4S					[M+Na] <sup>+</sup>	245.0589	
C00135		L-Histidine	C6H9N3O2					[M+H] <sup>+</sup>	156.0768	
C00020		Adenylic acid	C10H14N5O7P					[M+H] <sup>+</sup>	348.0704	

	C02759	alpha-Pinene-oxide	C10H16O					[M+K] <sup>+</sup>	191.0817
	C04435	(Z)-2-Methyl-5-isopropylhexa-2,5-dienal	C10H16O					[M+K] <sup>+</sup>	191.0817
<b>Limonene and pinene degradation</b>	C02676	Perillyl aldehyde	C10H14O					[M+Na] <sup>+</sup>	151.1119
	C01767	(-)-Carvone	C10H14O					[M+Na] <sup>+</sup>	151.1119
	C00964	(-)-trans-Carveol	C10H16O					[M+K] <sup>+</sup>	191.0817
	C02452	Perillyl alcohol	C10H16O					[M+K] <sup>+</sup>	191.0817
	C00521	(-)-Limonene	C10H16					[M+K] <sup>+</sup>	175.0869
		C01042	N-Acetyl-L-aspartate	C6H9NO5					[M-HCOOH+H] <sup>+</sup>
	C02362	2-Oxosuccinamate	C4H5NO4					[M+K] <sup>+</sup>	169.9862
	C00049	L-Aspartate	C4H7NO4					[M+H2O+H] <sup>+</sup>	152.0569
	C00152	L-Asparagine	C4H8N2O3					[M+H] <sup>+</sup>	133.0608
	C00402	D-Aspartate	C4H7NO4					[M+H2O+H] <sup>+</sup>	152.0569
	C03406	L-Argininosuccinate	C10H18N4O6					[M+H] <sup>+</sup>	291.1299
	C00041	L-Alanine	C3H7NO2					[M+H] <sup>+</sup>	90.0550
	C00026	2-Oxoglutarate	C5H6O5					[M+HCOONa] <sup>+</sup>	215.0166
	C00064	L-Glutamine	C5H10N2O3					[M+H] <sup>+</sup>	147.0764
	C00025	L-Glutamate	C5H9NO4					[M+H] <sup>+</sup>	148.0604
	C00334	gamma-Aminobutyric acid	C4H9NO2					[M+H] <sup>+</sup>	104.0706
	C00940	2-Oxoglutaramate	C5H7NO4					[M+K] <sup>+</sup>	184.0002
	C03912	L-1-Pyrroline-5-carboxylate	C5H7NO2					[M+H] <sup>+</sup>	114.0550
	C00042	Succinic acid	C4H6O4					[M+H] <sup>+</sup>	119.0339
	C00352	D-Glucosamine 6-phosphate	C6H14NO8P					[M+H] <sup>+</sup>	260.0530
	C03090	5-Phosphoribosylamine	C5H12NO7P					[M-CO+H] <sup>+</sup>	202.0476

Alanine, aspartate and glutamate metabolism