

Brain-dead and coma patients exhibit different serum metabolic profiles: a novel diagnostic approach in neurocritical care

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Table S1. List of assignments of ¹H NMR resonance signals with chemical shift, KEGG and HMDB ID. Presented in alphabetical order list of compounds that were used in multivariate and univariate analysis.

No.	Metabolite	Chemical shift	Multiplicity	HMDB ID	KEGG ID
1	3-Hydroxybutyrate	1.185	(d)	HMDB00357	C01089
2	3-Methyl-2-oxovalerate	1.107	(d)	HMDB00491	C03465
3	Acetate	1.904	(s)	HMDB00042	C00033
4	Acetoacetate	2.265	(s)	HMDB00060	C00164
5	Acetone	2.218	(s)	HMDB01659	C00207
6	Alanine	1.461	(d)	HMDB00161	C00041
7	Betaine	3.25	(s)	HMDB00043	C00719
8	Chol/PC/GPC	3.201	(m)	HMDB00097; HMDB00284; HMDB00086	C00114; C00588; C00670
9	Citrate	2.669	(dd)	HMDB00094	C00158
10	Creatine	3.029	(s)	HMDB00064	C00300
11	Creatinine	3.024	(s)	HMDB00562	C00791
12	Formate	8.441	(s)	HMDB00142	C00058
13	Glucose	3.232; 5.223	(m); (d)	HMDB00122	C00031
14	Glutamate	2.333	(m)	HMDB00148	C00025
15	Glutamine	2.427	(m)	HMDB00641	C00064
16	Glycine	3.54	(s)	HMDB00123	C00037
17	π -M-hist/ τ -M-hist	7.024	(s)	HMDB00479; HMDB00001	C01152
18	Methanol	3.347	(s)	-	-
19	π -M-hist/ τ -M-hist	7.726	(s)	HMDB00479; HMDB00001	C01152
20	Isobutyrate	1.055	(d)	HMDB01873	C02632
21	Isoleucine	0.991	(d)	HMDB00172	C00407

22	L 1	0.856	(m)	-	-
23	L 2	1.259	(m)	-	-
24	L 3	1.555	(m)	-	-
25	L 5	5.28	(m)	-	-
26	L_4 + NAC	2.027	(m)	-	-
27	Lactate	1.313; 4.101	(d); (q)	HMDB00190	C00186
28	Leucine	0.945	(t)	HMDB00687	C00123
29	Mannitol	3.67; 3.785	(m); (s)	HMDB00765	C00392
30	Mannose	5.171	(d)	HMDB00169	C00159
31	Phenylalanine	7.406	(m)	HMDB00159	C00079
32	Pyruvate	2.358	(s)	HMDB00243	C00022
33	Tyrosine	6.875	(m)	HMDB00158	C00082
34	Unk 1	1.158	(d)	-	-
35	Unk 2	1.169	(t)	-	-
36	Unk 3	1.284	(d)	-	-
37	Unk 4	1.913	(m)	-	-
38	Unk 5	2.06	(s)	-	-
39	Unk 6	2.148	(s)	-	-
40	Unk 7	2.903	(m)	-	-
41	Unk 8	3.164	(s)	-	-
42	Unk 9	7.138	(d)	-	-
43	Valine	0.969	(d)	-	-

Figure S1. Response permutation test plots for (A) the PLS-DA model (Table 1, Figure 2) and (B) OPLS-DA (Table 1, Figure 3); 500 permutations were used.

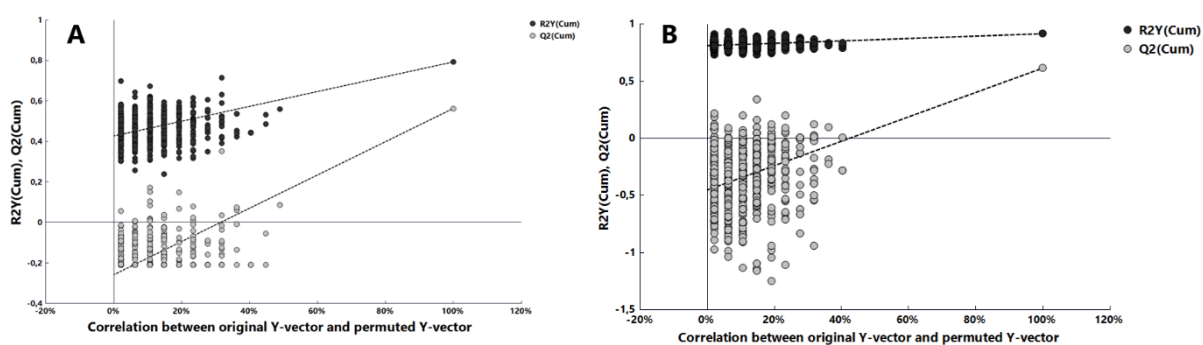


Figure S2. Pearson correlation heatmap for unassigned resonance signals.

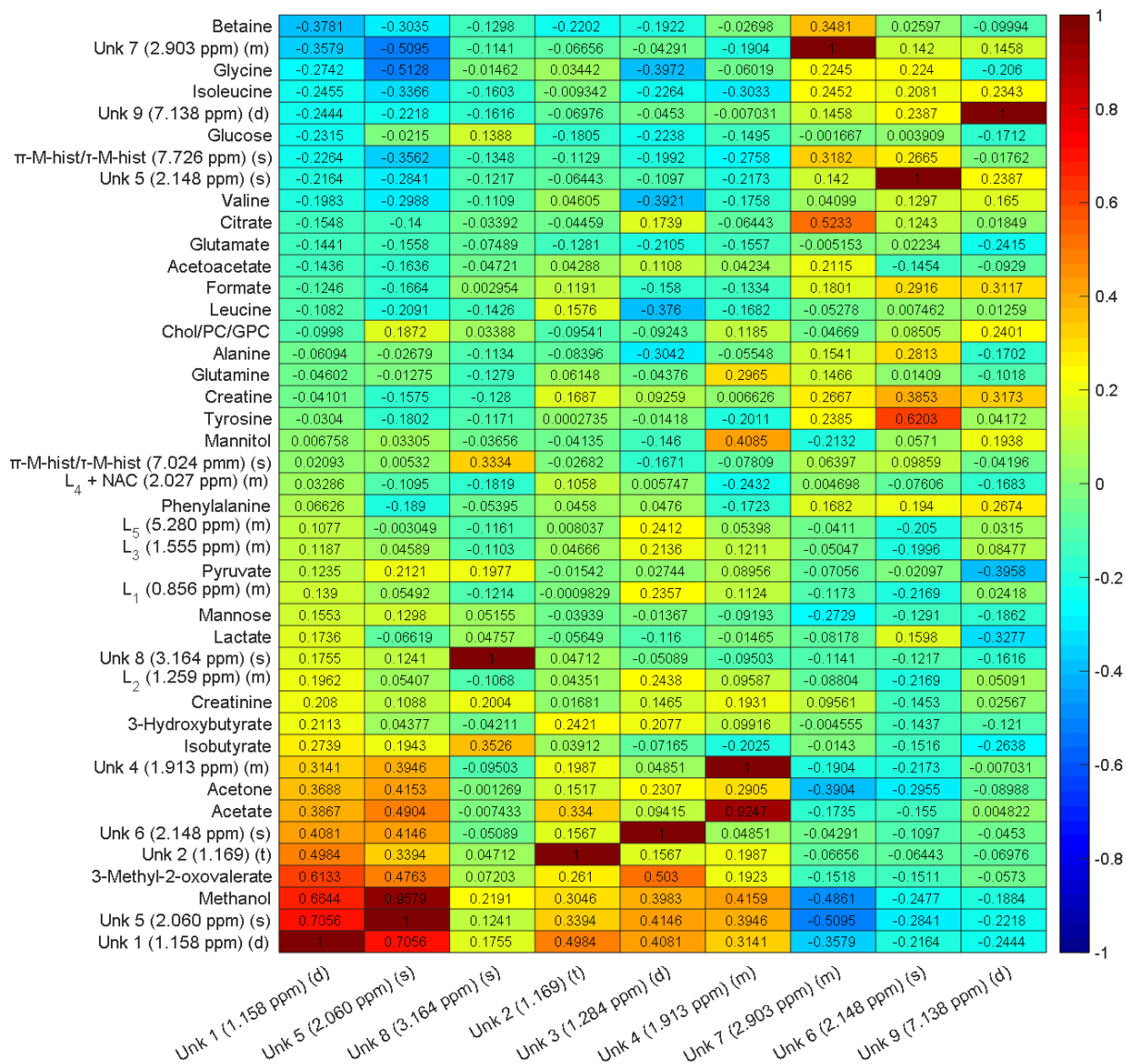


Figure S3. Cross-validated score plots for PLS-DA and OPLS-DA

