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Experimental Neurobiology

Supplementary Information

Title:

Metabolomic analysis identifies that amino acid metabolome signatures are altered in the postmortem brain of Alzheimer's disease

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Supple Table 2. Molecules of interest as identified by VIP value and p-value for their significance to the model.

No	RT	Mass	Detected method[a]	VIP value[b]	p-value	Fold change	Fold change direction	Name
1	1.24	148.0629	RP	9.15	1.28E-02	0.17	Down	Glutamate
2	1.42	103.0539	RP	8.47	6.49E-04	1.99	Up	2-Oxobutanoate
3	1.19	147.073	RP	7.31	4.86E-03	6.67	Up	4-Methylcatechol
4	1.13	90.0545	RP	6.85	2.25E-02	1.36	Up	Alanine
5	1.27	258.1094	RP	5.8	5.87E-03	2.99	Up	Pentahomomethionine
6	1.03	154.055	RP	5.74	2.17E-03	7.14	Up	Proline
7	0.96	191.0397	RP	5.4	1.88E-02	2.2	Up	Xanthine
8	1.67	152.0674	RP	5.24	1.83E-02	13.25	Up	5-Oxo-proline
9	1.3	86.096	RP	5.22	2.18E-02	1.74	Up	Piperidine
10	0.96	169.0577	RP	4.72	1.21E-02	2.83	Up	Acetylcholine
11	1.38	118.0648	RP	4.13	2.66E-04	1.97	Up	Valine
12	0.85	129.1381	RP	3.61	4.33E-02	1.48	Up	Unknown
13	1.18	175.0241	RN	3.56	4.80E-02	1.43	Up	Glucuronolactone
14	1.27	182.0806	RP	3.38	1.26E-02	1.87	Up	Tyrosine
15	1.21	184.0726	RP	3.12	2.53E-02	1.69	Up	Spermidine
16	1.7	247.1283	RP	3.07	2.40E-02	3.17	Up	N2-(D-1-Carboxyethyl)-arginine
17	1.42	95.0487	RP	2.95	7.26E-04	2.13	Up	Methylglyoxal
18	0.97	145.0616	RN	2.8	3.46E-02	1.48	Up	2-Oxoglutarate
19	0.93	296.0647	RP	2.72	2.14E-02	2.64	Up	Aminoimidazole ribotide
20	1.69	865.5025	HN	2.48	4.25E-02	0.6	Down	Unknown
21	1.27	327.0783	RP	2.32	3.75E-02	0.61	Down	N-Acetyl-aspartyl-glutamate
22	1	135.945	HN	2.32	2.15E-03	0.47	Down	Unknown
23	1.42	166.0789	RP	2.31	4.39E-04	1.91	Up	Formylanthranilate
24	1.67	110.0598	RP	2.28	2.73E-02	119.79	Up	Hypotaurine
25	10.98	363.2154	RP	2.26	9.95E-04	5.74	Up	Cortisol
26	0.8	625.5259	HN	2.26	3.39E-02	0.64	Down	Unknown
27	1.3	136.075	RP	2.26	1.63E-02	1.83	Up	Homocysteine
28	0.93	238.0438	RP	2.25	2.65E-04	2.1	Up	sn-glycero-3-Phosphoethanolamine
29	0.85	84.0802	RP	2.22	2.97E-02	1.46	Up	5-Aminoimidazole
30	9.52	590.9116	RP	2.18	6.27E-03	8.55	Up	Unknown
31	1.74	817.5035	HN	2.11	9.80E-04	0.39	Down	Unknown
32	0.91	214.0483	RN	2.11	1.16E-03	1.75	Up	Homophenylalanine
33	0.93	206.0543	RP	2.05	2.71E-03	1.9	Up	Xanthurenic acid
34	0.95	124.998	HN	2.05	3.41E-02	0.6	Down	Thymine
35	1.01	149.9933	HN	2.03	2.34E-02	0.61	Down	Guanine
36	0.82	73.5858	RP	1.99	1.52E-02	1.66	Up	Unknown
37	1.47	120.0714	RP	1.96	5.50E-04	1.96	Up	beta-Nitropropanoate

38	0.97	217.0291	RN	1.95	2.28E-04	1.74	Up	Sorbitol
39	9.34	238.1064	RP	1.87	5.90E-04	2.9	Up	Metanephrine
40	2.69	268.1031	HP	1.86	4.11E-02	0.46	Down	Deoxyguanosine
41	8.82	202.1075	RN	1.83	1.27E-02	1.87	Up	3-Methoxytyramine
42	1.69	841.5031	HN	1.78	2.00E-02	0.53	Down	Unknown
43	9.39	590.5111	RP	1.76	1.78E-02	35.03	Up	Unknown
44	1.72	819.5185	HN	1.75	6.99E-03	0.55	Down	Unknown
45	7.78	566.345	HN	1.71	1.92E-02	0.59	Down	Unknown
46	0.93	260.0255	RP	1.66	4.68E-04	2.05	Up	Glucosamine 6-phosphate
47	7.62	566.3522	HN	1.66	2.61E-02	0.6	Down	Unknown
48	7.26	156.9912	HN	1.65	2.38E-02	0.7	Down	(Z)-5-Oxohex-2-enedioate
49	9.52	591.11	RP	1.61	2.05E-02	8.66	Up	Unknown
50	3.84	181.0616	HN	1.57	2.31E-04	0.16	Down	Mannitol
51	8.39	498.0425	RP	1.56	4.41E-03	4.65	Up	2'-Deoxy-5-hydroxymethylcytidine-5'-triphosphate
52	9.37	236.0921	RN	1.55	2.42E-04	2.3	Up	6-Pyruvoyltetrahydropterin
53	0.96	203.052	RP	1.53	7.44E-04	2.25	Up	myo-Inositol
54	9.71	527.875	RP	1.5	9.65E-03	3.27	Up	Unknown
55	0.91	225.0614	RN	1.46	7.17E-03	1.42	Up	N-(omega)-Hydroxyarginine
56	9.25	313.1532	RP	1.46	2.04E-02	4.13	Up	N-(L-Arginino)succinate
57	1.14	132.111	RP	1.45	4.54E-02	1.39	Up	Bis(3-aminopropyl)amine
58	6.31	852.5785	HN	1.45	2.78E-03	0.65	Down	Unknown
59	1.47	166.1011	RP	1.44	2.44E-04	2.25	Up	Phenylalanine
60	8.8	204.1221	RP	1.4	4.26E-02	2.28	Up	9-Methylthiononanaldoxime
61	9.57	579.3082	RP	1.36	3.25E-02	9.52	Up	Unknown
62	9.44	455.255	RP	1.36	1.89E-02	3.34	Up	Secalciferol
63	1.32	305.0963	RP	1.34	4.36E-02	0.6	Down	Xylobiose
64	9.31	120.0802	RP	1.33	1.24E-04	2.8	Up	Threonine
65	4.7	555.2735	HN	1.32	2.78E-03	0.51	Down	Unknown
66	0.96	242.079	RN	1.31	3.71E-02	2.08	Up	N-Acetyl-L-phenylalanine
67	9.9	387.2474	RP	1.3	2.92E-02	1.11	Up	Urocortisone
68	8.32	454.7518	RP	1.28	1.81E-02	6.11	Up	Unknown
69	1.11	226.9957	RN	1.26	4.46E-02	1.37	Up	Citrate
70	1.32	303.0812	RN	1.24	2.72E-02	0.65	Down	Inosine
71	1.3	123.0435	RP	1.21	2.04E-02	1.71	Up	Nicotinamide
72	8.4	544.7739	RP	1.19	4.88E-04	4.44	Up	Unknown
73	9.13	475.324	RP	1.19	3.99E-02	0.81	Down	2-Phytyl-1,4-naphthoquinone
74	8.24	595.7711	RP	1.15	2.38E-02	2.03	Up	Unknown
75	5.18	173.9986	HN	1.14	2.25E-02	0.65	Down	N-Acetyl-L-aspartate
76	5.21	247.0118	HN	1.12	4.51E-02	0.66	Down	Pyridoxamine phosphate
77	8.93	558.0789	RP	1.08	1.78E-02	10.17	Up	Lipoyl-AMP
78	9.87	645.5838	RP	1.08	3.81E-03	3.58	Up	Unknown

79	1.45	102.046	RP	1.06	5.17E-04	2.13	Up	5-Aminopentanal
80	6.29	866.5823	HN	1.05	1.58E-02	0.7	Down	Unknown
81	9.55	579.7079	RP	1.04	3.02E-02	7.83	Up	Unknown
82	1.04	64.0138	RP	1.04	2.21E-02	1.58	Up	Unknown
83	9.78	268.9974	HP	1.03	4.27E-02	1.26	Up	Unknown
84	0.88	263.1098	RP	1.03	3.84E-02	0.31	Down	Homocarnosine
85	7.99	423.2583	RP	1.03	3.25E-02	3.7	Up	Desmosterol
86	0.9	128.9593	RN	1.02	3.26E-03	0.64	Down	2,2-Dichloro-1,1-ethanediol
87	9.12	745.7042	RP	1.01	1.05E-03	2.33	Up	Unknown
88	8.51	494.5391	RP	1.01	2.35E-03	5.13	Up	Unknown
89	7.98	245.1849	RP	1	2.40E-02	2.49	Up	Nerolidol

[a]Chromatographic methods and ionization methods for detection; RP : RPC-Positive mode, RN : RPC-Negative mode, HP : HILIC-Positive mode and HN : HILIC-Negative mode. [b]VIP value > 1 and p-value < 0.05 was used as cutoff value and all data sorted by VIP value.