

Supplementary Materials: Serum Metabolomic Profiling Identifies Characterization of Non-Obstructive Azoospermic Men

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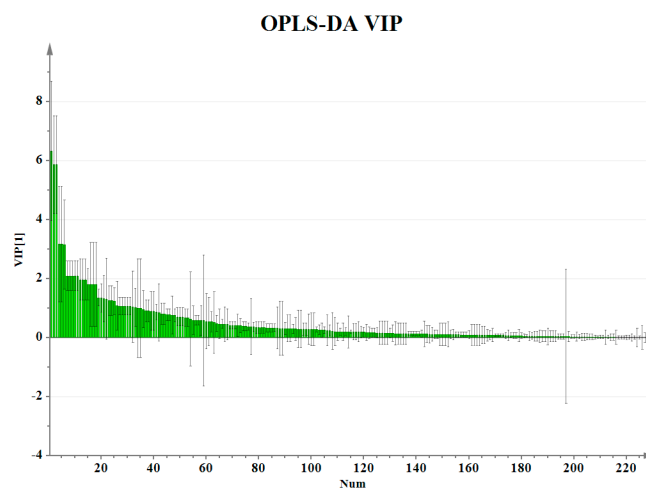


Figure S1. Variable influence on projection (VIP) of established orthogonal partial least squares-discriminant analysis (OPLS-DA) model. Variables with negative jack-knifing confidence intervals were eliminated.

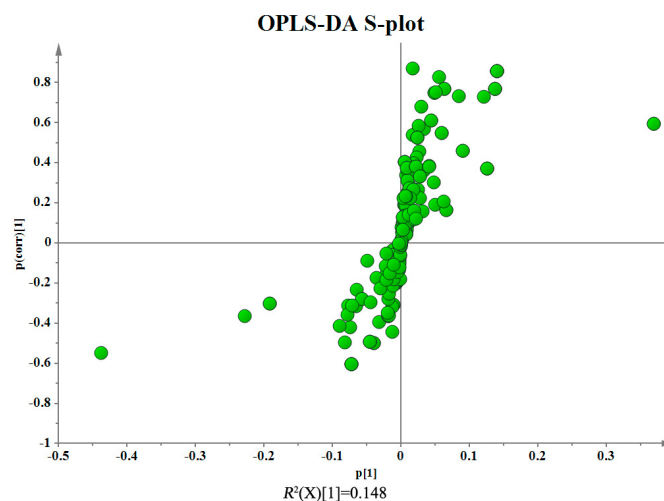


Figure S2. S-plot diagram of established OPLS-DA model. Variables that are closer to the lower-left and upper-right corners have greater contributions to group differentiation.

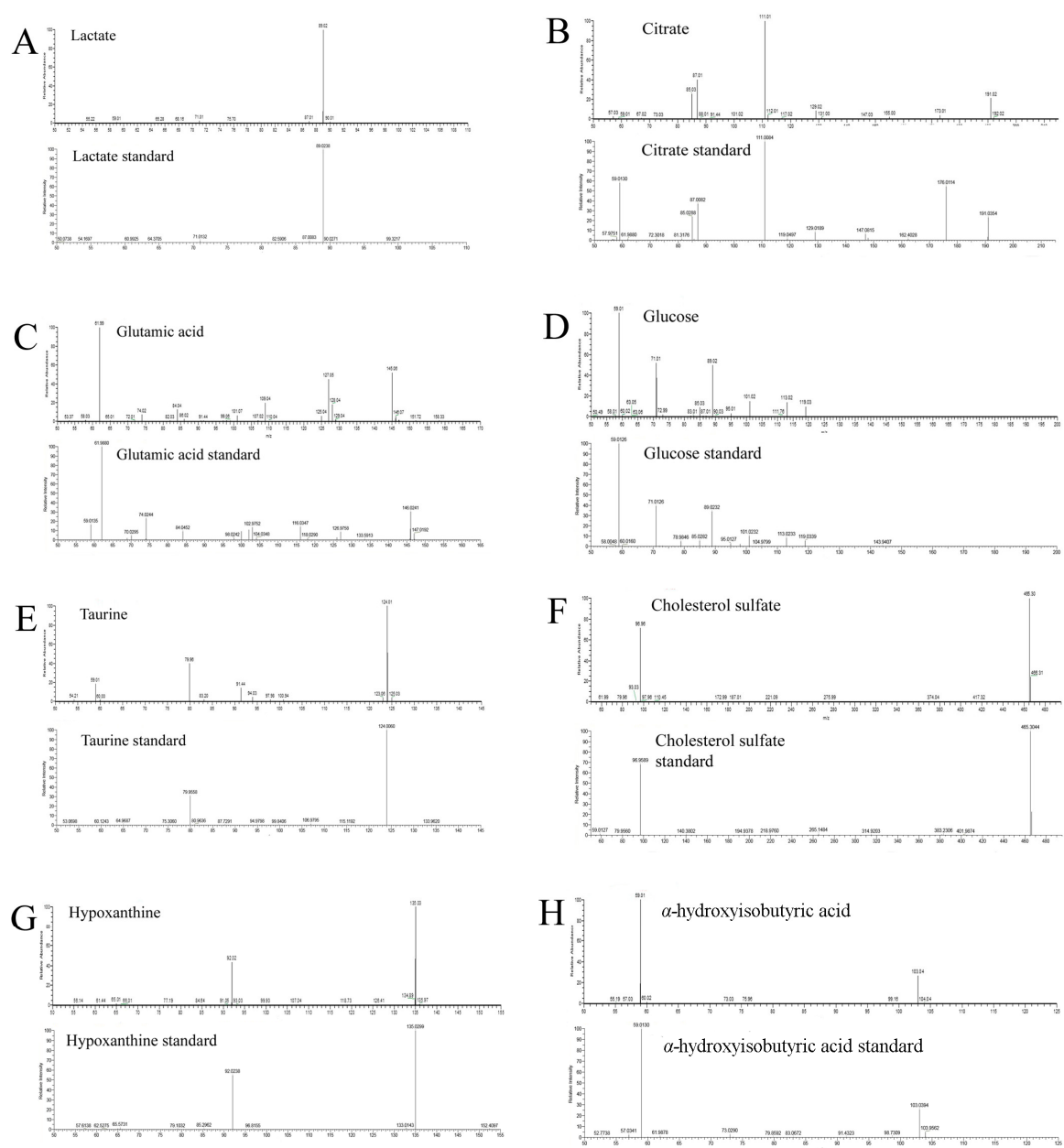


Figure S3. MS/MS spectra of lactate (A); citrate (B); glutamic acid (C); glucose (D); taurine (E); cholesterol sulfate (F); hypoxanthine (G); α -hydroxyisobutyric acid (H) in the serum of non-obstructive azoospermia with comparison to their standard.

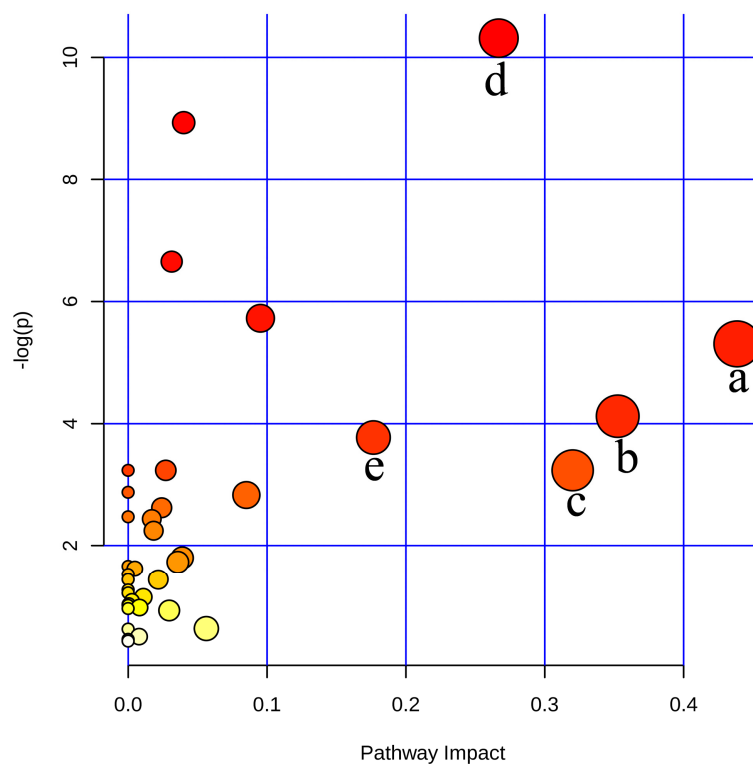


Figure S4. Metabolomics Pathway Analysis (MetPA) of disrupted serum metabolic pathway in patients with non-obstructive azoospermia. (a) D-glutamine and D-glutamate metabolism; (b) taurine and hypotaurine metabolism; (c) pyruvate metabolism; (d) the citrate cycle and (e) alanine, aspartate and glutamate metabolism.

Table S1. Disrupted serum metabolic pathway in patients with non-obstrucive azoospermia.

Metabolic Pathway	Total	Expected	Hits	Raw <i>p</i>	−log (Raw <i>p</i>)	Holm Adjust	FDR	Impact
D-Glutamine and D-glutamate metabolism	11	0.10968	2	0.004962	5.3059	0.37712	0.079393	0.4385
Taurine and hypotaurine metabolism	20	0.19942	2	0.016229	4.121	1	0.21639	0.35252
Pyruvate metabolism	32	0.31907	2	0.0394	3.234	1	0.3152	0.3201
Citrate cycle (TCA cycle)	20	0.19942	4	0.000033	10.314	0.002653	0.002653	0.26688
Alanine, aspartate and glutamate metabolism	24	0.2393	2	0.02301	3.7718	1	0.26297	0.17664
Glycolysis or Gluconeogenesis	31	0.3091	3	0.003261	5.7256	0.25113	0.065228	0.0953
Butanoate metabolism	40	0.39884	2	0.059048	2.8294	1	0.39366	0.08516
Aminoacyl-tRNA biosynthesis	75	0.74782	1	0.53393	0.62748	1	1	0.05634
Pentose and glucuronateinterconversions	53	0.52846	5	0.000132	8.9306	0.01045	0.005291	0.04002
Sulfur metabolism	18	0.17948	1	0.16558	1.7983	1	0.77921	0.03898
Arginine and proline metabolism	77	0.76776	2	0.17779	1.7272	1	0.79018	0.03582
Glyoxylate and dicarboxylate metabolism	50	0.49855	4	0.00129	6.6535	0.10058	0.034387	0.03137
Fatty acid metabolism	50	0.49855	1	0.39725	0.9232	1	0.9347	0.02959
Vitamin B6 metabolism	32	0.31907	2	0.0394	3.234	1	0.3152	0.02712
Ascorbate and aldarate metabolism	45	0.44869	2	0.072732	2.621	1	0.44758	0.02419
Valine, leucine and isoleucine biosynthesis	27	0.26921	1	0.23818	1.4347	1	0.79393	0.02173
Cysteine and methionine metabolism	56	0.55837	2	0.10595	2.2448	1	0.52974	0.01838
Starch and sucrose metabolism	50	0.49855	2	0.087346	2.4379	1	0.46585	0.01703
Glutathione metabolism	38	0.37889	1	0.31871	1.1435	1	0.93282	0.01095
Primary bile acid biosynthesis	47	0.46863	1	0.37847	0.97162	1	0.93282	0.00822
Purine metabolism	92	0.91732	1	0.60933	0.49539	1	1	0.00791
Selenoamino acid metabolism	22	0.21936	1	0.19863	1.6163	1	0.79393	0.00482
Galactose metabolism	41	0.40881	1	0.33922	1.0811	1	0.93282	0.00276
Histidine metabolism	44	0.43872	1	0.35913	1.0241	1	0.93282	0.00051

FDR, False Discovery Rate.