The urine metabolome of young autistic children correlates with the severity of clinical profile.
Supplementary Materials

Table S1. List of metabolites ruled out from statistical analysis

Valero lactam
5-Hydroxyhexanoic acid
3-Methylglutaconic acid
Ornithine lactam
Malic acid
Taurine
Anhydroglucose
3-Phosphoglycerate
Fructose
Chiroinositol
N-Acetylgalactosamine

Table S2. List of unknown metabolites recognized in this study by GC-MS.

Unknown 358 U	Sugar 1382
Unknown 794 U	Unknown 1457 U
U 807	Sugar 1602
Acid 823	Sugar 1624
Unknown 835 U	Monosacch E
Unknown 906 U	Sugar 1646
U D	U C
U 972	A231002
U 987	Monosacch 1886
A160001	U A
Unknown 1089 U	Unknown 1910
Sugar 1369	Disaccharide
A201005	

The urine metabolome of young autistic children correlates with the severity of clinical profile.
Supplementary Materials

Table S3. List of urine metabolites significantly correlating with scores computed by the Diagnostic Observation Schedule Second Edition with Calibrated Severity Score (ADOS-2 CSS)
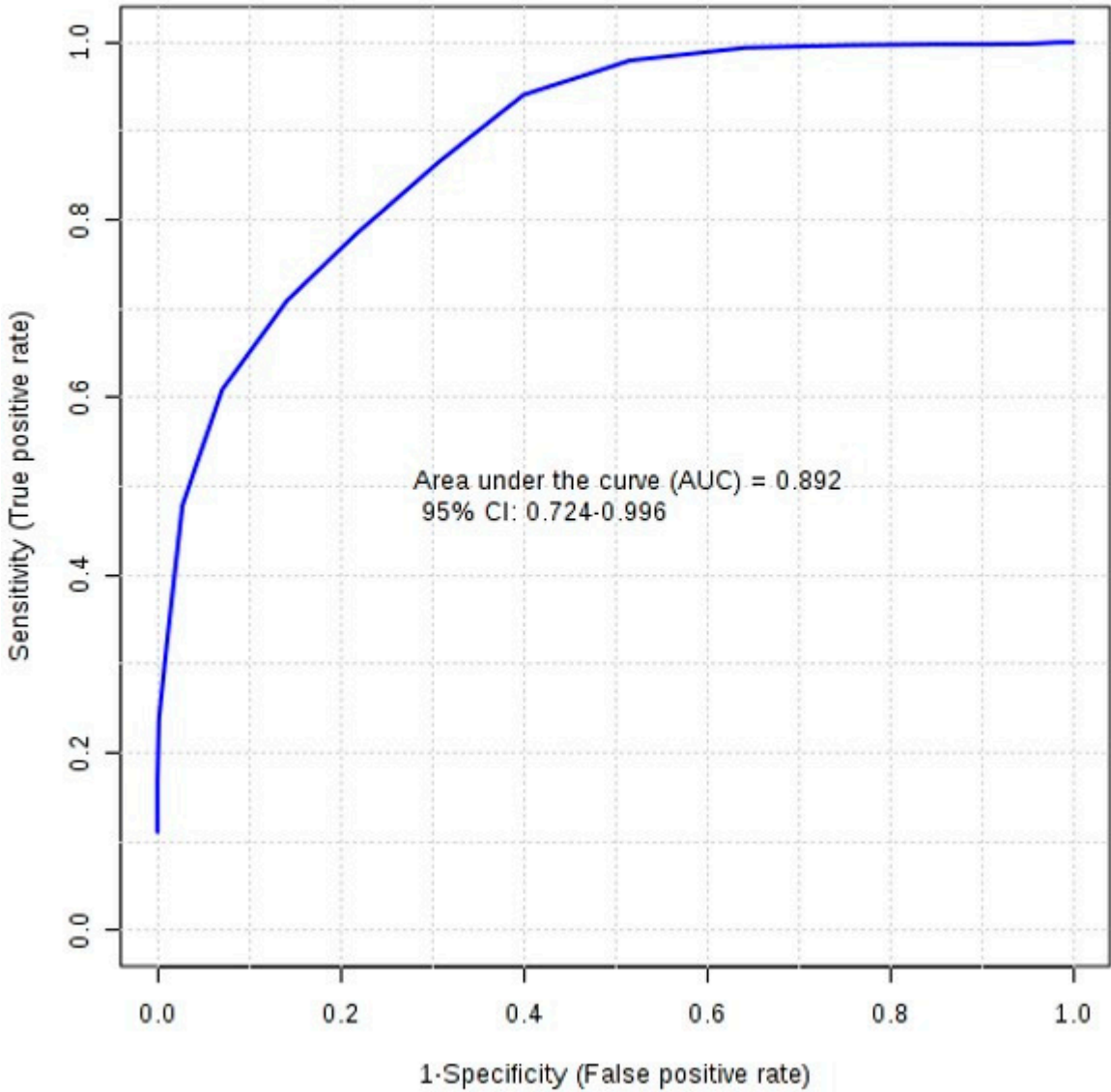
METABOLITE	SPEARMAN'S CORRELATION	
	ρ	*p*
2-Hydroxyacrylic acid	0.46	0.028
Allantoin	0.44	0.025
Adipic acid	050	0.023
3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid	0.46	0.020
Xylose	0.45	0.021
1-Deoxypentitol	0.45	0.020
Palmitic acid	0.65	0.003
Lyxonic acid	0.38	0.044
Quinolinic acid	0.43	0.033
Tri hydroxypentanoic acid	0.40	0.033

Table S4. Data matrix combining scores from RBS-R and ABC questionnaires with urine metabolome of ASD children

| URINE METABOLOME IDENTIFICATION	SCORE		URINE METABOLOME IDENTIFICATION	SCORE	
	RBS-R	ABC		RBS-R	ABC
Cluster 1 (n=11)			*Cluster 2 (n=20)*		
#69	15	18	#46	34	50
#27	24	80	#34	47	38
#61	65	70	#4	24	44
#28	51	59	#21	33	48
#37	9	34	#6	24	42
# 2	3	44	#23	35	50
#75	43	54	#30	8	17
#19	94	128	#55	17	32
#22	38	75	#33	31	81
#49	36	51	#67	19	45
#8	2	12	#58	35	23
			#15	36	46
			#11	12	23
			#85	4	10
			#60	39	94
			#13	2	4
			#71	35	49
			#39	6	49
			#7	23	38
			#10	23	29

Figure S1. ROC plot referred to the comparison between typically developed children and ASD children
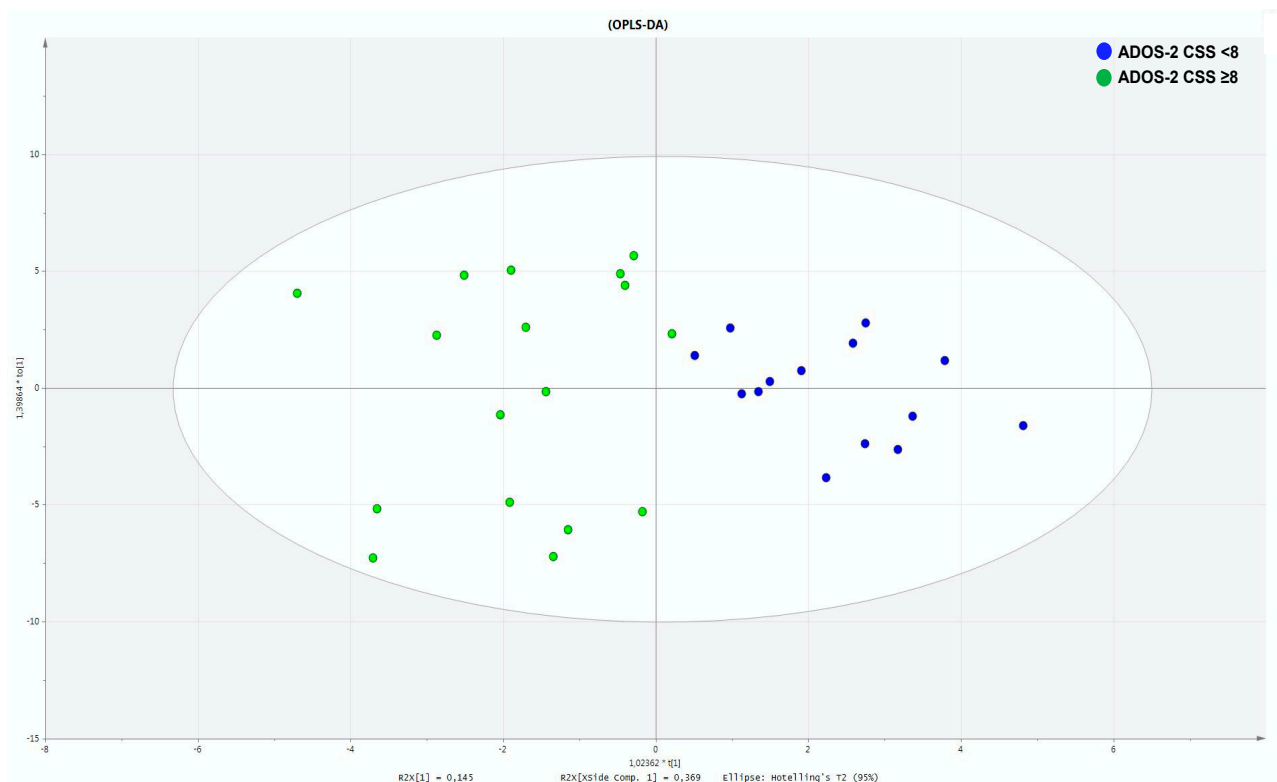
Figure S2. OPLS-DA score plot comparing the urine metabolic profile of the subgroup of ASD children with ADOS-2 CSS score ≥8 (blue dots) and that of ASD children with ADOS-2 CSS score <8 (red dots). The robustness of the model is supported by $R^2 X = 0.513$, $R^2 Y = 0.722$, $Q^2 = 0.468$ and confirmed by the analysis of variance CV-ANOVA (p=0.0092).