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Supplementary Materials for

A quasi-paired cohort strategy reveals the impaired detoxifying function of microbes in the gut of autistic children

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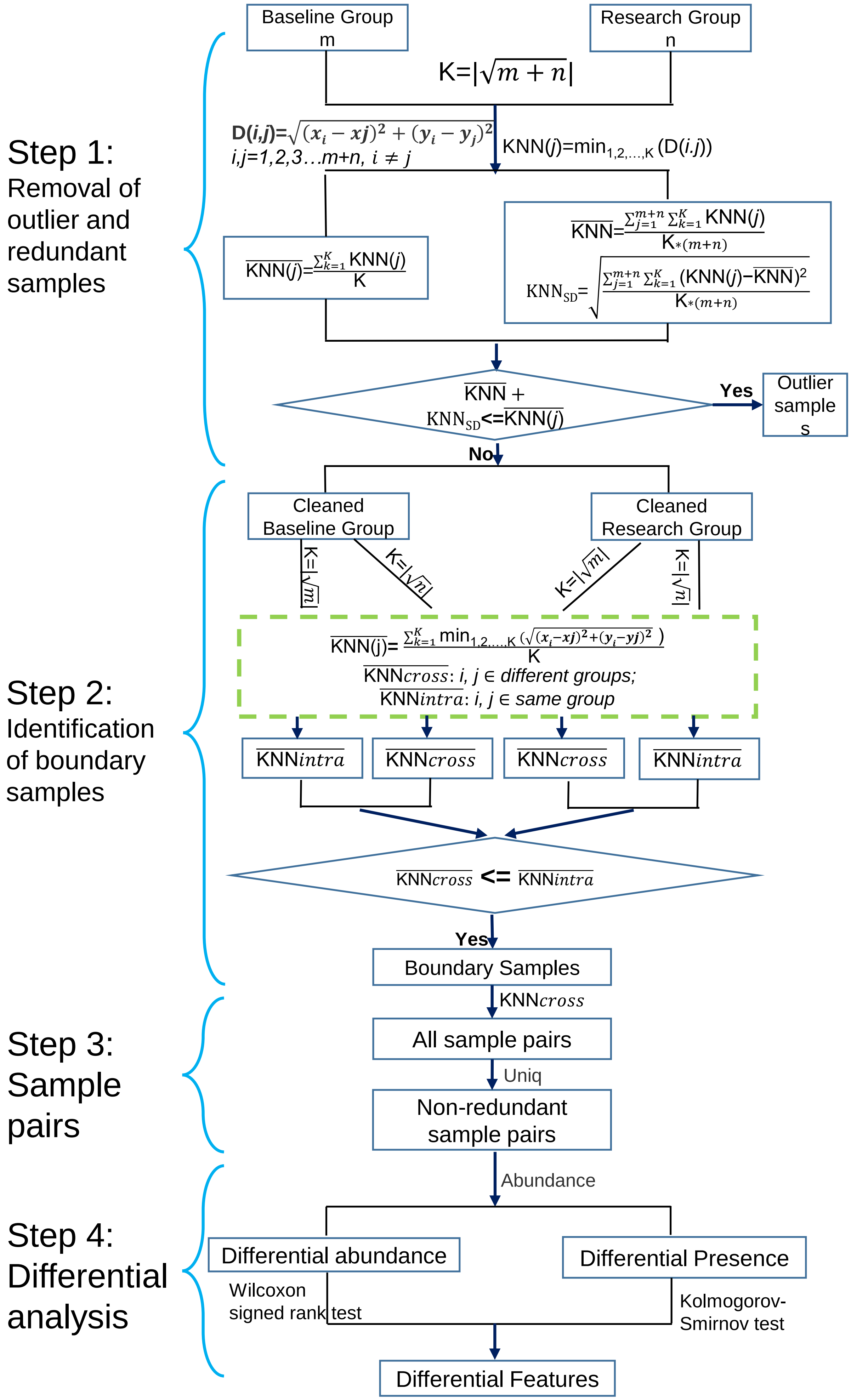

Fig. S1. Flowchart of quasi-paired cohort analysis

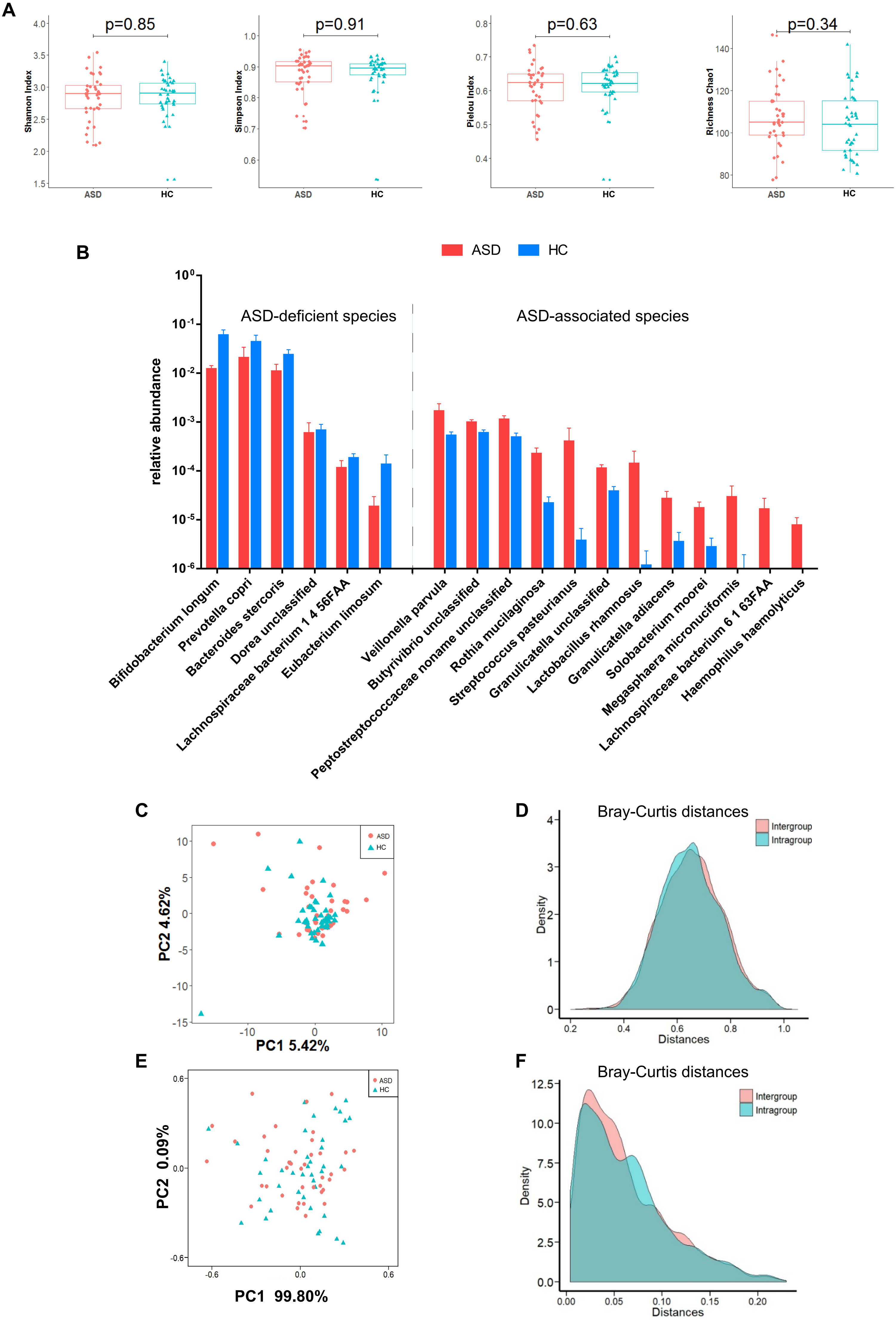
A
p=0.85
Shannon Index
ASD
HC
p=0.91
Simpson Index
p=0.63
Pielou Index
p=0.34
Richness Chao1
B
ASD
HC
relative abundance
ASD-deficient species
ASD-associated species
Bifidobacterium longum
Prevotella copri
Bacteroides stercoris
Dorea unclassified
Lachnospiraceae bacterium 1 4 56FAA
Eubacterium limosum
Veillonella parvula
Butyrivibrio unclassified
Peptostreptococcaceae noname unclassified
Rothia mucilaginosa
Streptococcus pasteurianus
Granulicatella unclassified
Lactobacillus rhamnosus
Granulicatella adiacens
Solobacterium moorei
Megasphaera micronuciformis
Lachnospiraceae bacterium 6 1 63FAA
Haemophilus haemolyticus
C
PC2 4.62%
PC1 5.42%
D
Bray-Curtis distances
Intergroup
Intragroup
Density
Distances
E
PC2 0.09%
PC1 99.80%
F
Bray-Curtis distances
Intergroup
Intragroup
Density
Distances

Fig. S2. Inter-individual diversity in intestinal microbiomes. A. Diversity and richness of the microbiome of ASD and HC, including the Shannon index, Simpson index, Pielou index and Chao1 richness. **B**. Differential species in HC and ASD samples. There are 6 deficient and 12 enriched species in ASD children (red) comparing with control subjects (blue) (Wilcoxon rank-sum test, $P<0.05$). Each bar represents the average relative abundance of a species. **C**. The principal coordinate analysis of species profile of the two groups. **D**. The Bray-Curtis distances of species profile of inter-group and intra-group sample pairs. **E**. The principal coordinate analysis of metabolic profile of the two groups. **F**. The Bray-Curtis distances of metabolic profile of inter-group and intra-group sample pairs.

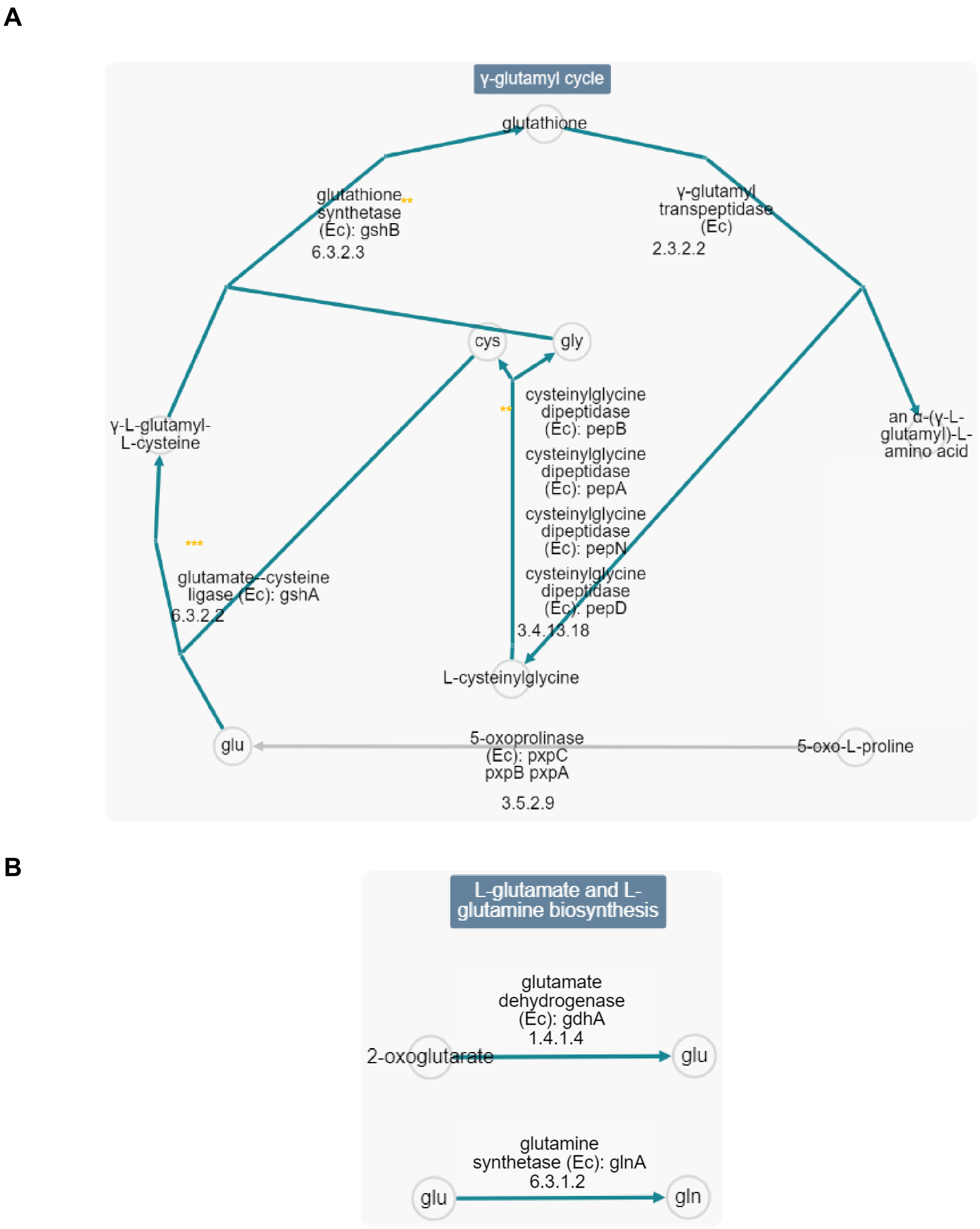

Fig. S3. Metabolic pathway of γ-glutamyl cycle (A) and biosynthesis of L-glutamate and L-glutamine (B). Green arrows, reactions with enzyme significantly deficient in ASD; gray arrows, reactions with enzyme showing no difference between ASD and HC. *P < 0.05,**P < 0.01, ***P < 0.001.

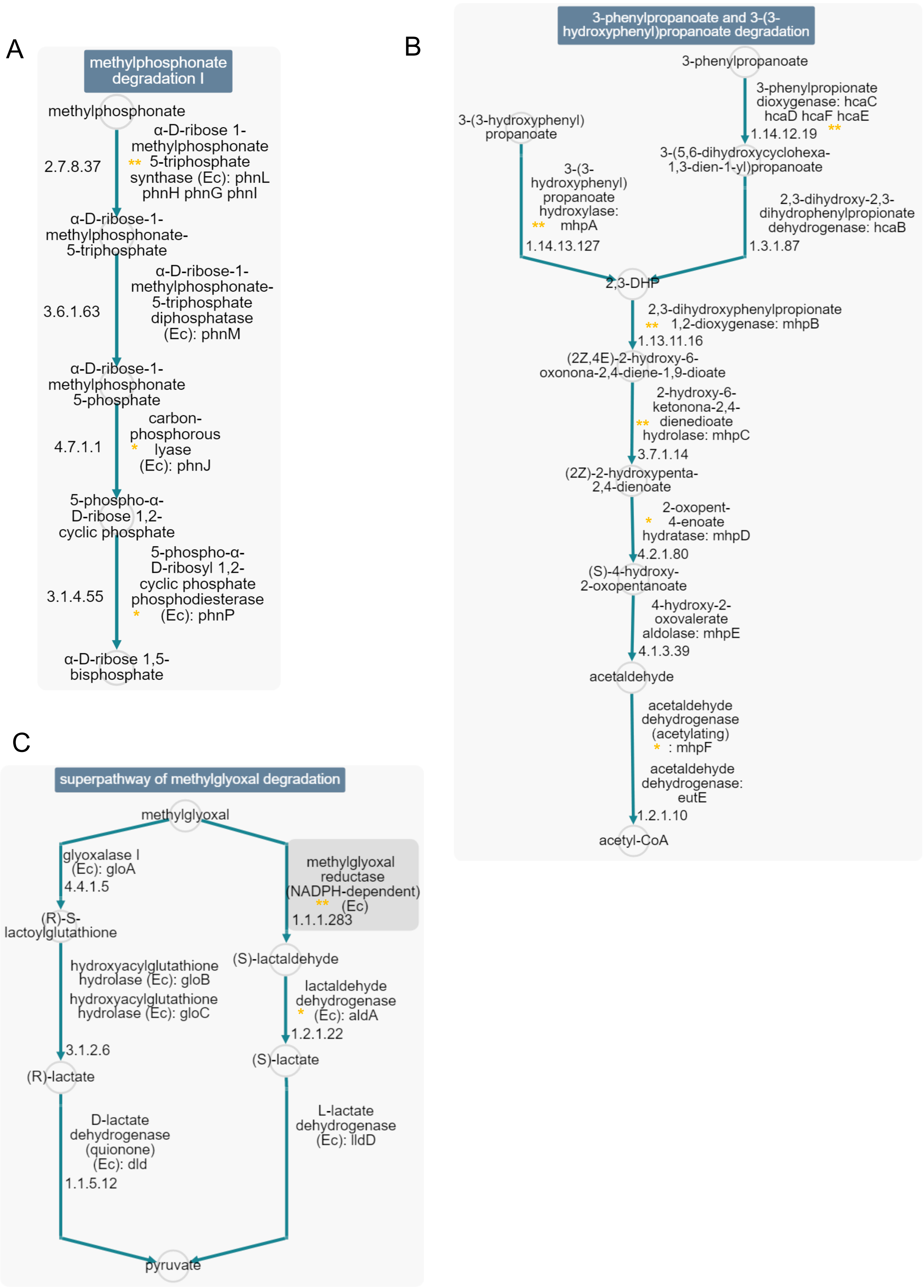

Fig.S4. Metabolic pathway of degradation of methylphosphonate (A), 3-phenylpropanoate or 3-(3-hydroxyphenyl)-propanoate (B), and methylglyoxal (C). See Fig.S3 for other legends

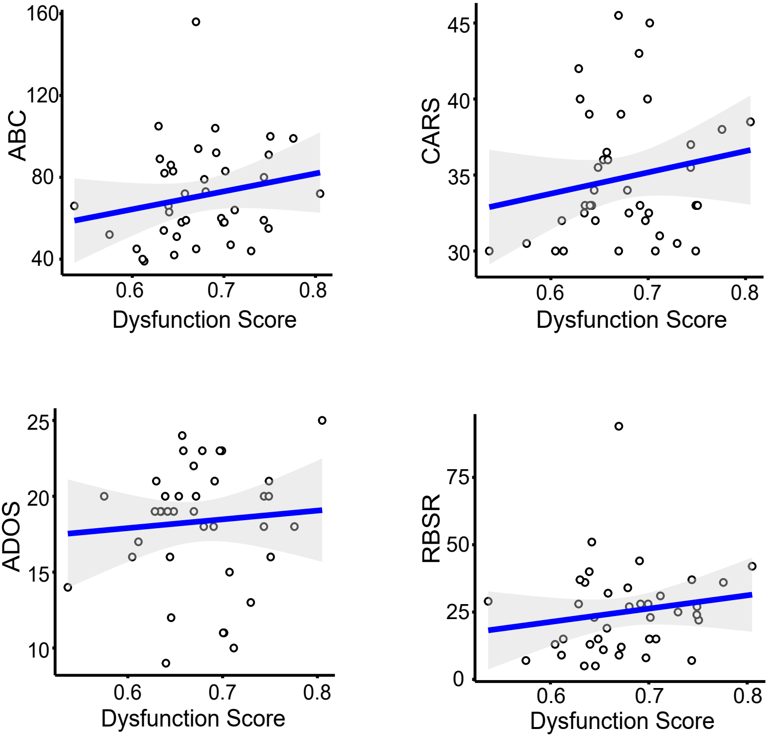

Fig. S5. Correlation between the dysfunction score and the clinical rating scores.

Table S1. Demographics of participants

	ASD(n=39)	HC(n=40)	P value
Age	5.57±1.09	5.61±1.24	0.8895
Body mass index	16.54±3.21	16.88±3.46	0.8682
Gender(n)			1
Female	7	7	
Male	32	33	
Type of delivery			0.0912
Vaginal	15	24	
Cesarean	24	16	
Falling asleep			0.0167*
Difficulty	15	5	
Non-difficulty	24	35	
Awaking in the midnight			0.0018**
Awoke	17	4	
Non-awoke	22	36	
ABC	70.90±23.75	NA	NA
GSI	3.97±2.54	NA	NA
RBS-R	25.03±16.56	NA	NA
CARS	34.82±4.33	NA	NA
ADOS	18.33±4.04	NA	NA

Table S2. ASD-associated pathways identified by quasi-paired cohort

Enrichment	Wilcoxon signed-rank paired test P-value	fdr	Pathways ID	Pathways Name
HC	0.000028	0.0033911	RIBOSYN2-PWY	flavin biosynthesis I (bacteria and plants)
HC	0.0000306	0.0033911	HEMESYN2-PWY	heme biosynthesis II (anaerobic)
HC	0.0001545	0.0137193	PWY-5189	tetrapyrrole biosynthesis II(from glycine)
HC	0.00046264	0.0319034	TEICHOICACID-PWY	teichoic acid poly glycerol biosynthesis
HC	0.00061637	0.0319034	PPGPPMET-PWY	ppGpp biosynthesis
HC	0.00064669	0.0319034	PRPP-PWY	superpathway of histidine purine and pyrimidine biosynthesis
HC	0.00076397	0.0339204	**PWY-4041**	**γ-glutamyl cycle**
HC	0.00091156	0.036794	KETOGLUCONMET-PWY	ketogluconate metabolism
HC	0.00152731	0.0474809	DAPLYSINESYN-PWY	L-lysine biosynthesis I
HC	0.001826	0.0474809	PWY-841	superpathway of purine nucleotides de novo biosynthesis I
HC	0.00190863	0.0474809	PWY-5656	mannosylglycerate biosynthesis I
HC	0.00262672	0.0485943	PWY-6731	starch degradation III
HC	0.00315144	0.0559696	**METHGLYUT-PWY**	**superpathway of methylglyoxal degradation**
HC	0.00379187	0.062849	PWY0-166	superpathway of pyrimidine deoxyribonucleotides de novo biosynthesis(E coli)
HC	0.00526401	0.062849	DENOVOPURINE2-PWY	superpathway of purine nucleotides de novo biosynthesis II
HC	0.00559166	0.062849	NAD-BIOSYNTHESIS-II	NAD salvage pathway II
HC	0.00607173	0.062849	PWY-6629	superpathway of L-tryptophan biosynthesis
HC	0.00729989	0.062849	PWY-6471	peptidoglycan biosynthesis IV (Enterococcus faecium)
HC	0.0073771	0.062849	PWY66-409	superpathway of purine nucleotide salvage
HC	0.00737885	0.062849	**HCAMHPDEG-PWY**	**3-phenylpropanoate and 3-(3-hydroxyphenyl)propanoate degradation to 2-oxopent-4-enoate**
HC	0.00737885	0.062849	**PWY-6690**	**cinnamate and 3-hydroxycinnamate degradation to 2-oxopent-4-enoate**
HC	0.00849072	0.062849	**PWY0-1277**	**3-phenylpropanoate and 3-(3-hydroxyphenyl)propanoate degradation**
HC	0.00894958	0.062849	PWY-7234	inosine-5-phosphate biosynthesis III
HC	0.00984291	0.062849	PWY-5989	stearate biosynthesis II (bacteria and plants)
HC	0.01041628	0.062849	PWY0-162	superpathway of pyrimidine ribonucleotides de novo biosynthesis
HC	0.0106139	0.062849	P161-PWY	acetylene degradation
HC	0.01088432	0.062849	ARGORNPROST-PWY	L-arginine degradation (Stickland reaction)
HC	0.01097858	0.062849	PWY-5705	allantoin degradation to glyoxylate III

HC	0.01122693	0.062849	FOLSYN-PWY	superpathway of tetrahydrofolate biosynthesis and salvage
HC	0.01122693	0.062849	PWY-7187	pyrimidine deoxyribonucleotides de novo biosynthesis II
HC	0.01143661	0.062849	**PWY0-1533**	methylphosphonate degradation I
HC	0.01203191	0.062849	PWY-7409	phospholipid remodeling phosphatidylethanolamine(yeast)
HC	0.01309857	0.0654768	PWY-7209	superpathway of pyrimidine ribonucleosides degradation
HC	0.01312485	0.0654768	PWY-7200	superpathway of pyrimidine deoxyribonucleoside salvage
HC	0.01411482	0.0695825	PWY-6901	superpathway of glucose and xylose degradation
HC	0.01426128	0.0695825	GLYCOLYSIS-E-D	superpathway of glycolysis and Entner Doudoroff
HC	0.01492186	0.0713288	PWY-6612	superpathway of tetrahydrofolate biosynthesis
HC	0.01676659	0.0791954	PWY-3841	folate transformations II
HC	0.01709177	0.0798815	PWY-7446	sulfoquinovose degradation I
HC	0.0175267	0.081061	PWY0-1261	anhydromuropeptides recycling I
HC	0.01831873	0.0823467	**PWY-5505**	L-glutamate and L-glutamine biosynthesis
HC	0.01864352	0.0823467	POLYISOPRENSYN-PWY	polyisoprenoid biosynthesis (E coli)
HC	0.01873202	0.0823467	AEROBACTINSYN-PWY	aerobactin biosynthesis
HC	0.01903636	0.0825077	PWY0-1338	polymyxin resistance
HC	0.01914031	0.0825077	PYRIDNUCSAL-PWY	NAD salvage pathway I
HC	0.01964961	0.0838887	PWY-6545	pyrimidine deoxyribonucleotides de novo biosynthesis III
HC	0.01999524	0.0845513	PWY0-1061	superpathway of L-alanine biosynthesis
HC	0.02034382	0.0852137	AST-PWY	L-arginine degradation II AST pathway
HC	0.02070212	0.0859041	FAO-PWY	fatty acid beta oxidation I
HC	0.02142999	0.0881011	PWY-6803	phosphatidylcholine acyl editing
HC	0.02180415	0.0888169	PWY-7184	pyrimidine deoxyribonucleotides de novo biosynthesis I
HC	0.02295614	0.0926593	PWY-5136	fatty acid beta oxidation II peroxisome
HC	0.02355153	0.0933336	PWY-5918	superpathay of heme biosynthesis from glutamate
HC	0.02375382	0.0933336	PWY-7197	pyrimidine deoxyribonucleotide phosphorylation
HC	0.02478339	0.0956698	PWY0-1297	superpathway of purine deoxyribonucleosides degradation
HC	0.02499442	0.0956698	PWY-7560	methylerythritol phosphate pathway II
HC	0.02499481	0.0956698	PWY-6270	isoprene biosynthesis I
ASD	0.00000327	0.0007267	RHAMCAT-PWY	L-rhamnose degradation I
ASD	0.00061637	0.0319034	NONOXIPENT-PWY	pentose phosphate pathway non oxidative branch
ASD	0.00188315	0.0474809	PWY-3781	aerobic respiration I cytochrome c
ASD	0.00208427	0.0474809	PWY-6737	starch degradation V
ASD	0.0022256	0.0474809	GLUCUROCAT-PWY	superpathway of beta D-glucuronide and D-glucuronate degradation
ASD	0.00224572	0.0474809	PWY-3801	sucrose degradation II sucrose synthase
ASD	0.00224572	0.0474809	PWY-7345	superpathway of anaerobic sucrose degradation

ASD	0.00495369	0.062849	POLYAMSYN-PWY	superpathway of polyamine biosynthesis I
ASD	0.00526415	0.062849	P125-PWY	superpathway of (R,R)-butanediol biosynthesis
ASD	0.00547651	0.062849	PWY-6837	fatty acid beta oxidation V unsaturated odd number di isomerase dependent
ASD	0.00617881	0.062849	GALACT-GLUCUROCAT-PWY	superpathway of hexuronide and hexuronate degradation
ASD	0.00695631	0.062849	PWY-6385	peptidoglycan biosynthesis III mycobacteria
ASD	0.0119759	0.062849	NADSYN-PWY	NAD biosynthesis II from tryptophan
ASD	0.0119759	0.062849	PWY-2201	folate transformations I
ASD	0.0119759	0.062849	PWY-5067	glycogen biosynthesis II (from UDP-D-Glucose)
ASD	0.0119759	0.062849	PWY-5079	L-phenylalanine degradation III
ASD	0.0119759	0.062849	PWY-5080	very long chain fatty acid biosynthesis I
ASD	0.0119759	0.062849	PWY-5304	superpathway of sulfur oxidation (Acidianus ambivalens)
ASD	0.0119759	0.062849	**PWY-5306**	superpathway of thiosulfate metabolism (Desulfovibrio sulfodismutans)
ASD	0.0119759	0.062849	PWY-5651	L-tryptophan degradation to 2-amino-3-carboxymuconate semialdehyde
ASD	0.0119759	0.062849	PWY-6074	zymosterol biosynthesis
ASD	0.0119759	0.062849	PWY-6075	ergosterol biosynthesis I
ASD	0.0119759	0.062849	PWY-6981	chitin biosynthesis
ASD	0.0119759	0.062849	PWY-7118	chitin degradation to ethanol
ASD	0.0119759	0.062849	PWY-7245	superpathway NAD/NADP - NADH/NADPH interconversion (yeast)
ASD	0.0119759	0.062849	PWY-7268	NAD/NADP-NADH/NADPH cytosolic interconversion (yeast)
ASD	0.0119759	0.062849	PWY-7283	wybutosine biosynthesis
ASD	0.0119759	0.062849	PWY-7286	7-(3-amino-3-carboxypropyl)-wyosine biosynthesis
ASD	0.0119759	0.062849	PWY-7288	fatty acid beta oxidation peroxisome (yeast)
ASD	0.0119759	0.062849	PWY-7411	superpathway of phosphatidate biosynthesis (yeast)
ASD	0.0119759	0.062849	PWY-7420	monoacylglycerol metabolism (yeast)
ASD	0.0119759	0.062849	PWY-7619	juniperonate biosynthesis
ASD	0.0119759	0.062849	PWY0-881	superpathway of fatty acid biosynthesis I (E coli)
ASD	0.0119759	0.062849	PWY3O-355	stearate biosynthesis III (fungi)
ASD	0.0119759	0.062849	TRIGLSYN-PWY	diacylglycerol and triacylglycerol biosynthesis
ASD	0.0119759	0.062849	UDPNACETYLGALSYN-PWY	UDP-N-acetyl-D-glucosamine biosynthesis II
ASD	0.01220453	0.0630094	PWY-6531	mannitol cycle
ASD	0.01282092	0.0654309	PWY-7279	aerobic respiration II cytochrome c (yeast)
ASD	0.01831873	0.0823467	PWY-5177	glutaryl-CoA degradation

Table S3. The metabolic categories of ASD-associated pathways

Function		**ASD-enriched**		**HC-enriched**	
Biosynthesis	**Amino Acid Biosynthesis**			PWY0-1061	superpathway of L-alanine biosynthesis
				PWY-5505	**L-glutamate and L-glutamine biosynthesis***
				DAPLYSINESYN-PWY	L-lysine biosynthesis I
				PWY-6629	superpathway of L-tryptophan biosynthesis
	Carbohydrate Biosynthesis/Cell Structure Biosynthesis	**PWY-6981**	**chitin biosynthesis (yeast)**	PWY-6471	peptidoglycan biosynthesis IV Enterococcus faecium
		PWY-5067	glycogen biosynthesis II (from UDP-D-Glucose)	TEICHOICACID-PWY	teichoic acid poly glycerol biosynthesis
		UDPNACETYLGALSYN-PWY	**UDP-N-acetyl-D-glucosamine biosynthesis II (yeast)**	PWY0-1338	polymyxin resistance
		PWY-6385	peptidoglycan biosynthesis III mycobacteria		
	Cofactor, Prosthetic Group, Electron Carrier, and Vitamin Biosynthesis	**PWY-7245**	**superpathway NAD/NADP - NADH/NADPH interconversion (yeast)**	NAD-BIOSYNTHESIS-II	NAD salvage pathway II
		PWY-7268	**NAD/NADP-NADH/NADPH cytosolic interconversion (yeast)**	PYRIDNUCSAL-PWY	NAD salvage pathway I
		NADSYN-PWY	NAD biosynthesis II from tryptophan	POLYISOPRENSYN-PWY	polyisoprenoid biosynthesis E coli
		PWY-2201	folate transformations I	HEMESYN2-PWY	heme biosynthesis II anaerobic
				PWY-5918	superpathay of heme biosynthesis from glutamate
				PWY-4041	**γ-glutamyl cycle**
				FOLSYN-PWY	superpathway of tetrahydrofolate biosynthesis and salvage
				PWY-6612	superpathway of tetrahydrofolate biosynthesis
				PWY-3841	folate transformations II
				RIBOSYN2-PWY	flavin biosynthesis I bacteria and plants

				PWY-5189	tetrapyrrole biosynthesis II from glycine
	Fatty Acid and Lipid Biosynthesis	**PWY-7420**	**monoacylglycerol metabolism (yeast)**	PWY-6803	phosphatidylcholine acyl editing
		TRIGLSYN-PWY	**diacylglycerol and triacylglycerol biosynthesis(yeast)**	PWY-5989	stearate biosynthesis II bacteria and plants
		PWY-5080	very long chain fatty acid biosynthesis I	**PWY-7409**	**phospholipid remodeling phosphatidylethanolamine (yeast)**
		PWY0-881	superpathway of fatty acid biosynthesis I E coli		
		PWY3O-355	**stearate biosynthesis III fungi/yeast**		
		PWY-7619	**juniperonate biosynthesis (yeast)**		
		PWY-7411	**superpathway of phosphatidate biosynthesis (yeast)**		
		PWY-6074	**zymosterol biosynthesis (yeast)**		
		PWY-6075	**ergosterol biosynthesis I (yeast)**		
	Purine / Pyrimidine Nucleotide Biosynthesis			PWY-7234	inosine-5-phosphate biosynthesis III
				PWY-841	superpathway of purine nucleotides de novo biosynthesis I
				DENOVOPURINE2-PWY	superpathway of purine nucleotides de novo biosynthesis II
				PWY66-409	superpathway of purine nucleotide salvage
				PWY0-166	superpathway of pyrimidine deoxyribonucleotides de novo biosynthesis E.coli
				PWY-7187	pyrimidine deoxyribonucleotides de novo biosynthesis II
				PWY-6545	pyrimidine deoxyribonucleotides de novo biosynthesis III
				PWY-7184	pyrimidine deoxyribonucleotides de novo biosynthesis I
				PWY0-162	superpathway of pyrimidine ribonucleotides de novo biosynthesis
				PWY-7200	superpathway of pyrimidine deoxyribonucleoside salvage

				PWY-7197	pyrimidine deoxyribonucleotide phosphorylation
				PRPP-PWY	superpathway of histidine purine and pyrimidine biosynthesis
	Secondary Metabolite Biosynthesis			AEROBACTINSYN-PWY	aerobactin biosynthesis
				PWY-6270	isoprene biosynthesis I
				PWY-7560	methylerythritol phosphate pathway II
	Metabolic Regulator Biosynthesis			PPGPPMET-PWY	ppGpp biosynthesis
				PWY-5656	mannosylglycerate biosynthesis I
	Amine and Polyamine Biosynthesis	POLYAMSYN-PWY	superpathway of polyamine biosynthesis I		
Degradation/Utilization /Assimilation	**Carbohydrate/Carboxylate Degradation**	PWY-6737	starch degradation V	PWY-6731	starch degradation III
		RHAMCAT-PWY	L-rhamnose degradation I	PWY-6901	superpathway of glucose and xylose degradation
		PWY-3801	sucrose degradation II sucrose synthase	P161-PWY	acetylene degradation
		PWY-7345	superpathway of anaerobic sucrose degradation	KETOGLUCONMET-PWY	ketogluconate metabolism
		PWY-5177	glutaryl-CoA degradation		
		GLUCUROCAT-PWY	superpathway of β-D-glucuronosides degradation		
	Amino Acid Degradation	**PWY-5079**	**L-phenylalanine degradation III (yeast)**	ARGORNPROST-PWY	L-arginine degradation (Stickland reaction)
		PWY-5651	**L-tryptophan degradation to 2-amino-3-carboxymuconate semialdehyde**	AST-PWY	L arginine degradation II AST pathway
	Aromatic Compound Degradation			**PWY0-1277**	**3-phenylpropanoate and 3-(3-hydroxyphenyl)propanoate degradation**
				HCAMHPDEG-PWY	**3-phenylpropanoate and 3-(3-hydroxyphenyl)propanoate degradation to 2-oxopent-4-enoate**
				PWY-6690	**cinnamate and 3-hydroxycinnamate degradation to 2-oxopent-4-enoate**
	Fatty Acid and Lipid Degradation	**PWY-6837**	**fatty acid beta-oxidation V (yeast)**	FAO-PWY	fatty acid beta oxidation I

		PWY-7288	**fatty acid β-oxidation (peroxisome, yeast)**	PWY-5136	fatty acid beta oxidation II peroxisome
	Inorganic Nutrient Metabolism	**PWY-5306**	**superpathway of thiosulfate metabolism** Desulfovibrio sulfodismutans	**PWY0-1533**	**methylphosphonate degradation I**
		PWY-5304	superpathway of sulfur oxidation Acidianus ambivalens		
	Nucleoside and Nucleotide Degradation			PWY0-1297	superpathway of purine deoxyribonucleosides degradation
				PWY-7209	superpathway of pyrimidine ribonucleosides degradation
	Secondary Metabolite Degradation	PWY-6531	mannitol cycle	PWY0-1261	anhydromuropeptides recycling I
				PWY-7446	sulfoquinovose degradation I
	Aldehyde Degradation			**METHGLYUT-PWY**	**superpathway of methylglyoxal degradation**
	Allantoin Degradation			PWY-5705	allantoin degradation to glyoxylate III
Generation of Precursor Metabolite and Energy		**PWY-7118**	**chitin degradation to ethanol (yeast)**	GLYCOLYSIS-E-D	superpathway of glycolysis and the Entner-Doudoroff pathway
		PWY-7279	**aerobic respiration II cytochrome c (yeast)**		
		P125-PWY	superpathway of (R,R)-butanediol biosynthesis		
		NONOXIPENT-PWY	pentose phosphate pathway non oxidative branch		
		PWY-3781	aerobic respiration I cytochrome c		
Macromolecule Modification	**Nucleic Acid Processing**	**PWY-7283**	**wybutosine biosynthesis (yeast)**		
		PWY-7286	7-(3-amino-3-carboxypropyl)-wyosine biosynthesis		

Table S4. ASD-deficient enzymes involved in toxicant degradation.

EC number	Enzyme	Gene	pathway	substrate	meanASD	meanHC	Wilcoxon signed-rank paired test P-value	fdr
3.6.1.7	acylphosphatase; acetylphosphatase	yccX	Aminobenzoate degradation	Benzoyl phosphate	2.29E-05	3.91E-05	2.72E-05	0.003035
4.1.1.61	4-hydroxybenzoate decarboxylase	ECO26_3806/ECO26_3807	Aminobenzoate degradation	phenol	4.86E-07	2.43E-06	0.033416	0.10691
3.5.1.4	amidase; acylamidase; acylase	gatA	Aminobenzoate degradation; Styrene degradation	Benzamide；Phenylacetamide; Acrylamide	1.04E-07	1.77E-07	0.000188	0.010585
2.8.3.6	3-oxoadipate CoA-transferase	pcaI(Escherichia fergusonii)	Benzoate degradation	3-oxoadipate	1.76E-08	5.02E-08	0.002705	0.043417
1.14.12.10	benzoate 1,2-dioxygenase; benzoate hydroxylase	benA(Escherichia fergusonii)	Benzoate degradation	benzoate	2.26E-08	3.34E-08	0.002768	0.043727
1.1.1.1	alcohol dehydrogenase; aldehyde reductase	adhP/yiaY	Chloroalkane and chloroalkene degradation; Naphthalene degradation	Chloro-2-propene-1-ol;Chloroallyl alcohol;2-Naphthaldehyde	3.84E-05	4.90E-05	0.020169	0.075624
1.2.1.39	phenylacetaldehyde dehydrogenase	feaB	Styrene degradation	Phenylacetaldehyde	3.24E-07	9.55E-07	0.043549	0.12847
1.1.1.90	aryl-alcohol dehydrogenase	KPN_01945(Klebsiella pneumoniae)	Xylene degradation	Methylbenzyl alcohol	4.43E-08	1.03E-07	0.0023	0.04055

Table S5. Measurements of urine organic acids in ASD children

Urinal organic acid	meanASD	meanHC	enrich group	wilcoxon text p-value	fdr
N-Acetylcysteine	0.144231	0.087667	ASD	5.77E-05	0.004328
2-Hydroxyphenylacetic acid	1.407692	0.701667	ASD	0.000491	0.010956
Suberic acid	4.847692	2.643333	ASD	0.00067	0.010956
2-Oxo-4-methiolbutyric acid	0.135769	0.105444	ASD	0.002119	0.020093
Mandelic acid	0.118077	0.076111	ASD	0.002143	0.020093
Sebacic acid	0.189615	0.127611	ASD	0.002949	0.022116
Phoshoric acid	4621.577	2635.056	ASD	0.003302	0.022514
Thymine	0.428846	0.294056	ASD	0.005202	0.028812
2-Oxoisovaleric acid	1.031154	0.736111	ASD	0.005378	0.028812
Fumaric acid	1.551538	0.901111	ASD	0.006265	0.031327
Glutaric acid	1.668077	0.928889	ASD	0.01177	0.049043
2-Hydroxyhippuric acid	0.967308	0.524056	ASD	0.013466	0.051474
2-Hydroxyisovaleric acid	0.299231	0.274611	ASD	0.013788	0.051474
Methylsuccinic acid	3.716154	2.512778	ASD	0.014413	0.051474
2-Oxoisocaproic acid	0.217692	0.174778	ASD	0.019554	0.063764
Aconitic acid	26.96462	18.26	ASD	0.025612	0.080037
5-HIAA	4.614615	4.020556	ASD	0.035656	0.102873
Glycolic acid	45.42308	23.10056	ASD	0.035663	0.102873
4-Hydroxyhippuric acid	20.79346	14.57833	ASD	0.037806	0.105016
Carboxycitric acid	12.28038	8.685556	ASD	0.041165	0.106683
Pantothenic acid	3.822692	2.832222	ASD	0.041251	0.106683
N-Acetylaspartic acid	2.550385	1.866111	ASD	0.046218	0.115545
α-Oxoglutaric acid	27.275	19.775	ASD	0.057673	0.135172
3-Methylgutaric acid	0.946154	0.634278	ASD	0.060935	0.137474
Phenyllactic acid	0.167692	0.106278	ASD	0.062321	0.137474
4-Cresol	19.81692	14.02278	ASD	0.077295	0.165631
Pyridoxic acid	20.99423	18.98667	ASD	0.132554	0.26162
Ascorbic acid	53.55769	48.59556	ASD	0.145322	0.272479
5-Hydroxymethyl-2-furoic acid	12.65808	9.470556	ASD	0.155376	0.277588
Pyroglutamic acid	46.65269	33.27778	ASD	0.155449	0.277588
2-Hydroxybutyric acid	0.902308	0.619056	ASD	0.166119	0.28326
Oxalic acid	51.71923	46.71056	ASD	0.166179	0.28326
Tricarballylic acid	1.042692	0.878333	ASD	0.185125	0.308492
Vanillylmandelic(VMA)	6.727308	5.431111	ASD	0.189209	0.308492
Benzoic acid	3.097692	2.923333	ASD	0.197301	0.314842
Succinic acid	17.05077	14.18556	ASD	0.2101	0.321582
2-Hydroxyisocaproic acid	0.245769	0.203111	ASD	0.236442	0.354662
Creatinine	0.748462	0.632222	ASD	0.242074	0.355991
Adipic acid	5.861923	4.764444	ASD	0.251851	0.356654
HMG	21.49962	19.58833	ASD	0.256791	0.356654
Malic acid	2.423846	2.121667	ASD	0.310295	0.408283
Homegentisic acid	0.203846	0.195389	ASD	0.396054	0.495068
Quinolinic acid	3.278462	3.157778	ASD	0.410172	0.50431
DHPPA	0.508846	0.35	ASD	0.56654	0.663914

3-Indoleacetic acid	5.910769	4.093333	ASD	0.582977	0.671441
Citric acid	82.25	76.91111	ASD	0.693672	0.753991
Homovanillic(HVA)	7.889231	6.857222	ASD	0.792871	0.837539
Methylmalonic acid	2.699231	2.633333	ASD	0.95241	0.961907
Glyceric acid	1.894231	3.933889	HC	0.000196	0.007352
Citramalic acid	1.073846	2.467778	HC	0.00073	0.010956
Ethylmalonic acid	2.012308	5.789444	HC	0.001168	0.014598
4-Hydroxyphenylacetic acid	11.12538	24.58389	HC	0.002432	0.020268
4-Hydroxyphenyllactic acid	0.396154	0.909444	HC	0.004321	0.027006
3-Oxoglutaric acid	0.192308	0.375556	HC	0.007166	0.03359
Phenylpyruvic acid	1.512692	3.374389	HC	0.008946	0.039469
Furan-2,5-dicarboxylic acid	6.332308	9.353333	HC	0.01754	0.059794
Lactic acid	8.77	16.03833	HC	0.057167	0.135172
HVA/VMA-ratio	1.166538	1.431111	HC	0.083401	0.173753
Malonic acid	4.606154	6.502222	HC	0.104511	0.211847
Hippuric acid	130.5154	195.5111	HC	0.138867	0.267052
3-Methyl-2-oxovaleric acid	0.45	0.451111	HC	0.205311	0.320798
Pyruvic acid	1.825385	2.526667	HC	0.256774	0.356654
4-Hydroxybenzoic acid	0.918077	1.148722	HC	0.288043	0.392786
Orotic acid	0.446154	0.689556	HC	0.293341	0.392868
Uracil	3.942692	6.512778	HC	0.339652	0.439205
Hydroxybutyric acid	2.235769	2.661111	HC	0.37709	0.479352
HPHPA	43.22269	46.70722	HC	0.515478	0.623563
Quinolinic acid/5-HIAA	0.753462	0.820556	HC	0.526943	0.627313
Arabinose	19.47077	23.235	HC	0.590868	0.671441
Kynurenic acid	1.174615	1.599444	HC	0.658708	0.735888
Tartaric acid	2.641538	2.944444	HC	0.667205	0.735888
4-Hydroxybutyric acid	1.473846	1.743889	HC	0.711359	0.76217
Acetoacetic acid	3.640769	3.896111	HC	0.820553	0.854743
Furancarbonylglycine	1.262692	1.73	HC	0.914422	0.939475
Methylcitric acid	1.785769	2.386111	HC	0.961907	0.961907