Figure S1

A

B

Significant shifted between ASD and NT

- Total ASD score (severity)
- Repetitive behavior
- Social retardation
- Language retardation
- Total GI problem score (severity)
Figure S3

A. Mean relative abundance of *Veillonella ratti* (OTU 359954)

B. Mean relative abundance of *Enterobacter* (OTU 2119418)

C. Mean relative abundance of *Clostridium* (OTU 182289)
Figure S4

A. Inner (-) subjects among PC1 outer (+)

B. Inner (-) subjects among PC2 outer (+)

C. Inner (-) subjects among PC3 outer (+)

D. Validation cohort 1

E. Validation cohort 2

Physiological age
Figure S5

A

B

C

Gut, et al. Lou M.
Figure S6

A. Microbial co-occurrence network alteration between NT and ASD before 3y

B. Microbial co-occurrence network alteration between NT and ASD after 3y

C. Before 3y → After 3y
Microbial community alteration network in NT

D. Before 3y → After 3y
Microbial community alteration network in ASD

E. NT0 NT1 l1r abundance scatter, PM score: 0.077

F. ASD0 ASD1 l1r abundance scatter, PM score: 0.516
Figure S7

A

**Relative abundance of Veillonella (%)**

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B

Veillonella correlations with other taxon in NT0

C

Veillonella correlations with other taxon in NT1

D

Veillonella correlations with other taxon in ASD0

E

Veillonella correlations with other taxon in ASD1
Figure S8

A

B

GBM - clinical phenotype

METACYC - clinical phenotype
Figure S9

A. Significant associations (−log(qval)*sign(coef))

- Veillonella
- Lachnospira
- Hungatella
- uncultured Lachnospiraceae NK4A136 group
- _L_Ruminococcaceae_
- Faecalibacterium
- Blautia
- Lachnospiraceae UCG004
- Granulicatella
- _L_Enterobacteriaceae_
- Flavonifractor
- Clostridium sensu stricto 1

B. Significant associations (−log(qval)*sign(coef))

- MGB041. fumarate pathway
- MGB053. Butyrate synthesis II
- MGB015. p Cresol synthesis
- MGB027. NO oxigenase
- MGB023. Dopamine degradation
- MGB007. Glutamate synthesis II
- MGB043. Acetate synthesis I
- MGB056. Propionate degradation I
- MGB050. Glutamate degradation I
- MGB036. SAM synthesis
- MGB019. GABA degradation
- MGB048. Propionate synthesis I
- MGB004. Kyurenine synthesis

C. Significant associations (−log(qval)*sign(coef))

- PWY 7090. UDP-2,3-diacetamido-2,3-dideoxy-b-D-mannuronate biosynthesis
- PWY 5897. superpathway of menaquinol 11 biosynthesis
- PWY 5898. superpathway of menaquinol 12 biosynthesis
- PWY 5899. superpathway of menaquinol 13 biosynthesis
- PWY 5838. superpathway of menaquinol 8 biosynthesis I
- PWY 7003. glycerol degradation to butanol
- PWY 7332. superpathway of UDP-N-acetylglucosamine derived O-antigen building blocks biosynthesis
- GLUTORN PWY. L-ornithine biosynthesis
- PANTOSYN PWY. pantothene and coenzyme-A biosynthesis I
- THRESYN PWY. superpathway of L-threonine biosynthesis
- PWY 6471. peptidoglycan biosynthesis IV Enterococcus faecium
- ARGSYN PWY. L-arginine biosynthesis I via L-ornithine
- NONMEVIPP PWY. methylethylthiol phosphate pathway I
- PWY 7560. methylethylthiol phosphate pathway II
- PWY 7400. L-arginine biosynthesis IV archaeabacteria
- PWY 6163. chorismate biosynthesis from 3 dehydroquininate
- PWY 6470. peptidoglycan biosynthesis V b-lactam resistance
- HEME BIOSYNTHESIS II. heme biosynthesis I aerobic
- COA PWY. coenzyme-A biosynthesis I
- PWY 3001. superpathway of L-isoleucine biosynthesis I
- PWY 5188. tetrapyrrole biosynthesis I from glutamate
- PWY0 1061. superpathway of L-alanine biosynthesis
- GLCMANNANAU PWY. superpathwa of N-acetylglucosamine, N-acetylmannosamine and N-acetylenuraminic degradation
- PWY 5189. tetrapyrrole biosynthesis II from glycine
- PWY 5918. superpathway of heme biosynthesis from glutamate
- PWY 5505. L-glutamate and L-glutamine biosynthesis
- X1MET2 PWY N10. formyl tetrahydrofolate biosynthesis
- PWY 621. sucrose degradation III sucrose invertase
Figure S10

A. Top 20 factors in subjects ≤ 3 y (current cohort)

B. Current cohort (≤3y)

C. Top 20 factors in subjects > 3 y (current cohort)

D. Current cohort (>3y)

E. Validation cohort 1

F. Validation cohort 1

G. Validation cohort 2

H. Validation cohort 2

I. Validation cohort 3

J. Validation cohort 3

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Figure S11

A. Validation cohort 1

B. Validation cohort 2

C. Validation cohort 3

Normalized relative abundance

Legend:
- ASD
- NT

Significance:
* p < 0.05
** p < 0.01
*** p < 0.001

Sample IDs:
- PWY-3027
- PWY-3036
- PWY-3046
- PWY-3055
- PWY-3065
- PWY-3075
- PWY-3085
- PWY-3095
- PWY-3105
- PWY-3115
- PWY-3125
- PWY-3135
- PWY-3145
- PWY-3155

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