

Supplementary Table S1. Most abundant genera in control (MAG0) and their strains % distribution.

Genus	AVD	LpxA	LpxC	LpxD	LpxH	LpxB	LpxK	WaaA	LpxL	LpxM
<i>Bacteroides</i>	40.1988	2.39	96.06	91.96	2.38	62.68	98.26	0	100	100
<i>Alistipes</i>	13.1825	3.08	93.02	95.45	4.26	48.89	95.35	100	0	0
<i>Faecalibacterium</i>	5.4047	0	0	0	0	0	0	0	0	0
<i>Parabacteroides</i>	4.4801	2.71	96	98.28	0.6	64.41	98.31	100	0	0
<i>Dialister</i>	2.3337	17.65	88.24	92.86	0	40	88.24	0	0	0
<i>Sutterella</i>	1.6737	19.79	64.52	100	80.95	100	89.47	0	0	0
<i>Oscillibacter</i>	1.4705	0	0	0	0	0	0	0	0	0
<i>Bacteroidales_noname</i>	1.1350	61.52	69.64	37.5	44.44	19.35	56.9	0	0	0
<i>Odoribacter</i>	1.0652	16.67	100	84.62	0	11.11	100	0	0	0
<i>Prevotella</i>	1.0291	4.57	97.33	65.55	2.52	54.55	98.51	0	0	0
<i>Blautia</i>	0.9643	0	0	0	0	0	0	0	0	0
<i>Akkermansia</i>	0.8059	6.49	81.25	87.5	0	15.79	75	0	0	0
<i>Paraprevotella</i>	0.7158	2.44	75	75	0	66.67	100	0	0	0
<i>Bilophila</i>	0.6073	12.5	100	100	0	0	100	0	0	0
<i>Lachnospiraceae_noname</i>	0.5326	0.67	0	0	0	100	100	0	0	0

Abbreviations: AVD, average value distribution.

Supplementary Table S2. Most abundant genera in ASD (MAG) and their strains % distribution.

Genus	AVD	LpxA	LpxC	LpxD	LpxH	LpxB	LpxK	WaaA	LpxL	LpxM
<i>Bacteroides</i>	43.9726	2.39	96.06	91.96	2.38	62.68	98.26	0	100	100
<i>Alistipes</i>	14.7629	3.08	93.02	95.45	4.26	48.89	95.35	100	0	0
<i>Faecalibacterium</i>	4.2211	0	0	0	0	0	0	0	0	0
<i>Parabacteroides</i>	2.8816	2.71	96	98.28	0.6	64.41	98.31	100	0	0
<i>Dialister</i>	2.4613	17.65	88.24	92.86	0	40	88.24	0	0	0
<i>Oscillibacter</i>	2.1972	0	0	0	0	0	0	0	0	0
<i>Lachnospiraceae_noname</i>	1.5793	0.67	0	0	0	100	100	0	0	0
<i>Akkermansia</i>	1.5705	6.49	81.25	87.5	0	15.79	75	0	0	0
<i>Blautia</i>	1.1117	0	0	0	0	0	0	0	0	0
<i>Haemophilus</i>	0.8035	14.75	51.19	98.92	90.48	99.04	99	96.88	49.18	50.83
<i>Bacteroidales_noname</i>	0.7764	61.52	69.64	37.5	44.44	19.35	56.9	0	0	0
<i>Prevotella</i>	0.6930	4.57	97.33	65.55	2.52	54.55	98.51	0	0	0
<i>Sutterella</i>	0.5924	19.79	64.52	100	80.95	100	89.47	0	0	0
<i>Escherichia</i>	0.5787	4.91	43.43	85.53	49.5	93.91	96.42	100	31.18	43.63
<i>Odoribacter</i>	0.5664	16.67	100	84.62	0	11.11	100	0	0	0

Abbreviations: AVD, average value distribution; ASD, autism spectrum disorder.

Supplementary Table S3. Most increased genera (MIG) and their strains % distribution.

Genus	AVD-CN	AVD-ASD	%Increase	LpxA	LpxC	LpxD	LpxH	LpxB	LpxK	WaaA	LpxL	LpxM
<i>Acidaminococcus</i>	8.86E-05	0.0057	6409.81	19.05	57.14	87.5	0	62.5	80	0	0	0
<i>Megasphaera</i>	0.0053	0.1523	2774.09	11.11	100	100	0	71.43	95.45	100	0	0
<i>Porphyromonas</i>	0.0002	0.0042	1352.23	6.93	100	100	4.35	34.88	100	100	100	0
<i>Klebsiella</i>	0.0134	0.1672	1144.98	5.56	49.21	97.73	50.56	89.94	97.18	100	45.8	27.08
<i>Burkholderiales_noname</i>	0.0608	0.4617	658.58	9.51	46.46	90.91	34.88	88.46	90.2	100	0	0
<i>Citrobacter</i>	0.0007	0.0034	383.44	5.45	47.52	83.33	52.94	95.08	95.95	100	31.38	34.44
<i>Neisseria</i>	0.0008	0.0039	354.85	13.03	48.42	98.11	94.23	97.12	97.98	100	100	0
<i>Actinobacillus</i>	0.0004	0.0017	242.33	13.44	52.08	88.46	96.15	88.89	92.31	100	51.02	51.06
<i>Enterobacter</i>	0.0802	0.2407	199.98	6.53	48.35	52	95	95.2	98.61	100	44.16	25.78
<i>Lachnospiraceae_noname</i>	0.5326	1.5793	196.52	0.67	0	0	0	100	100	0	0	0

Abbreviations: AVD, average value distribution; ASD, autism spectrum disorder; CN, control.

Supplementary Table S4. Most abundant species in control and individuals with ASD.

SPECIES	AVD-CN	SPECIES	AVD-ASD
<i>Bacteroides uniformis</i>	8.2699	<i>Bacteroides uniformis</i>	9.1107
<i>Alistipes putredinis</i>	6.7517	<i>Bacteroides vulgatus</i>	6.3990
<i>Bacteroides vulgatus</i>	5.7016	<i>Alistipes onderdonkii</i>	6.0277
<i>Faecalibacterium prausnitzii</i>	5.4047	<i>Alistipes putredinis</i>	5.0361

<i>Bacteroides dorei</i>	3.9207	<i>Bacteroides ovatus</i>	4.4489
<i>Bacteroides ovatus</i>	3.3417	<i>Faecalibacterium prausnitzii</i>	4.2212
<i>Bacteroides massiliensis</i>	3.3369	<i>Bacteroides cellulosilyticus</i>	3.8806
<i>Bacteroides caccae</i>	3.0294	<i>Bacteroides dorei</i>	2.9137
<i>Bacteroides plebeius</i>	2.8978	<i>Bacteroides caccae</i>	2.7306
<i>Alistipes onderdonkii</i>	2.7979	<i>Dialister invisus</i>	2.4613
<i>Barnesiella intestinihominis</i>	2.5968	<i>Bacteroides massiliensis</i>	2.1281
<i>Parabacteroides merdae</i>	2.2584	<i>Bacteroides fragilis</i>	2.1123
<i>Dialister invisus</i>	2.1834	<i>Bacteroides stercoris</i>	2.1052
<i>Bacteroides cellulosilyticus</i>	1.8241	<i>Alistipes finegoldii</i>	1.5904
<i>Sutterella wadsworthensis</i>	1.6737	<i>Akkermansia muciniphila</i>	1.5705
<i>Alistipes shahii</i>	1.5342	<i>Bacteroides thetaiotaomicron</i>	1.5166
<i>Bacteroides fragilis</i>	1.3903	<i>Alistipes shahii</i>	1.3599
<i>Bacteroides thetaiotaomicron</i>	1.3552	<i>Barnesiella intestinihominis</i>	1.3320
<i>Bacteroides stercoris</i>	1.1828	<i>Parabacteroides merdae</i>	1.1630

Abbreviations: AVD, average value distribution; ASD, autism spectrum disorder; CN, control.

Supplementary Table S5. Most increased species and their strains % distribution.

Species	AVD-CN	AVD-ASD	% Increase	LpxA	LpxC	LpxD	LpxH	LpxB	LpxK	WaaA	LpxL	LpxM
<i>Klebsiella oxytoca</i>	0.0005	0.0377	6253	6.91	40.91	90.91	51.85	92.86	100	100	32.43	35.14
<i>Bacteroides clarus</i>	0.0205	0.6414	3020	1.67	100	100	0	33.33	100	0	0	0
<i>Acidaminococcus fermentans</i>	8.86E-05	0.0026	2931	21.43	66.67	66.67	0	66.67	66.67	0	0	0
<i>Escherichia unclassified</i>	0.0027	0.0558	1964	5.2	46.58	86.75	51.16	97.23	100	100	32.38	51.16
<i>Bacteroides intestinalis</i>	0.0480	0.6447	1243	1.41	1	1	0	47.06	85.71	0	0	0
<i>Klebsiella pneumoniae</i>	0.0125	0.1259	904	7.21	68.35	98.7	63.56	92.22	100	92.11	50.27	28.48
<i>Bacteroides faecis</i>	0.0770	0.7648	892	3.7	100	100	0	33.33	60	0	0	0
<i>Citrobacter freundii</i>	0.0003	0.0024	602	8.57	36	87.5	50	48.39	92.5	100	56.9	64.91
<i>Haemophilus sputorum</i>	0.0031	0.0107	245	16.67	50	100	100	100	100	0	50	50
<i>Desulfovibrio piger</i>	0.0179	0.0550	207	0	0	0	0	0	0	0	0	0
<i>Oxalobacter formigenes</i>	0.0014	0.0042	202	10	50	100	100	100	100	0	0	0
<i>Alistipes unclassified</i>	0.1135	0.3160	178	3.08	93.02	95.45	4.26	48.89	95.35	100	0	0
<i>Phascolarctobacterium succinatutens</i>	0.2166	0.5515	155	15.79	100	100	0	100	100	0	0	0
<i>Akkermansia muciniphila</i>	0.8059	1.5705	95	6.61	100	90	0	18.18	83.33	0	0	0
<i>Bacteroides stercoris</i>	1.1828	2.1052	78	3.7	100	100	5.88	85.71	92.86	100	0	0
<i>Bilophila wadsworthia</i>	0.0333	0.0559	68	12.5	100	100	0	100	100	0	0	0
<i>Alistipes senegalensis</i>	0.0197	0.0327	66	0	0	0	0	0	0	0	0	0
<i>Bilophila unclassified</i>	0.1884	0.2985	58	12.5	100	100	0	0	100	0	0	0
<i>Bacteroides coprocola</i>	0.0460	0.0706	54	3.57	100	100	0	66.67	100	100	0	0
<i>Bacteroides fragilis</i>	1.3903	2.1123	52	0.94	100	96.15	2	81.58	100	100	0	0

Abbreviations: AVD, average value distribution; ASD, autism spectrum disorder; CN, control.