Supplementary Table 1

Ulcerative colitis (n=49)	
Site of disease	
Total (%)	22 (44.9%)
Rectal (%)	8 (16.3%)
Left (%)	19 (38.8%)
Matts Endoscopy Score	
1	24 (49.0%)
2	14 (28.6%)
3	6 (12.2%)
4	5 (10.2%)
Clinical Activity Index	
0 – 3	38 (22.4%)
4 $\leqq$	11 (77.6%)
UC Drugs	
Anti-TNF antibody	1 (2.0%)
Immunosuppressant	11 (22.4%)
Prodrug of 5-ASA	34 (69.4%)
PPI	7 (14.3%)
Steroid	7 (14.3%)
Probiotics	40 (81.6%)

Supplementary Table 1. UC patient information (Study 1).

The number and ratio of patients with different lesion sites, disease severity score, or drug treatments.

Supplementary Table 2

Crohn's Disease (n = 40)	
Site of disease	
Small Intestine (%)	13 (32.5 %)
Colon (%)	4 (10 %)
Both (%)	23 (57.5 %)
Modified Rutgeerts score	
0-1 (remission)	12 (30 %)
2-4 (active)	28 (70 %)
CDAI	
<150	30 (75 %)
150 – 220	6 (15 %)
220 – 300	2 (5 %)
300<	2 (5 %)
CD Drugs	
Anti-TNF antibody	23 (57.5 %)
Immunosuppressant	13 (32.5 %)
Prodrug of 5-ASA	34 (85.0%)
PPI	1 (2.5 %)
Antibiotics	2 (5.0 %)
Probiotics	27 (67.5 %)

Supplementary Table 2. CD patient information (Study 1).

The number and ratio of patients with different lesion sites, disease severity score, or drug treatments.

Supplementary Table 3

	Sia	Gal	Fuc	GlcNAc	GalNAc	Man	Ara	Rib	Xyl	Rha
mol%										
Healthy	2.4 ± 1.1	24.1 ± 2.8	4.4 ± 0.9	28 ± 4.9	11.4 ± 2.5	1.0 ± 1.0	11.7 ± 2.5	4.1 ± 4.1	13.0 ± 3.3	0 ± 0
UC	1.7 ± 0.5	31.4 ± 6.4	16.6 ± 8.3	18.4 ± 1.9	7.8 ± 1.6	5.0 ± 3.3	8.3 ± 2.5	0 ± 0	10.7 ± 2.1	0 ± 0

Supplementary Table 3. Sugar compositions in stool glycans of Healthy subjects and UC patients.
Sugar compositions in stool glycans of healthy subjects and UC patients. Data represent the mean ±
standard deviation (n = 3/group).

Supplementary Table 4

Organic acids	Healthy (*n* = 43)	UC		CD	
		Active (*n* = 25)	Remission (*n* = 24)	Active (*n* = 10)	Remission (*n* = 30)
Acetate	43 (100%)	25 (100%)	24 (100%)	10 (100%)	10 (100%)
Propionate	43 (100%)	47 (96%)	24 (100%)	8 (80%)	10 (100%)
n-Butyrate	43 (100%)	16 (64%)	20 (83%)	5 (50%)	24 (80%)
Lactate	6 (14%)	5 (20%)	5 (21%)	3 (30%)	5 (17%)
Succinate	30 (70%)	11 (44%)	11 (46%)	4 (40%)	14 (47%)
i-Valerate	9 (21%)	6 (12%)	2 (8.3%)	2 (20%)	7 (23.3%)
n-Valerate	7 (16%)	0 (0%)	0 (0%)	1 (10%)	2 (6.7%)
i-Butyrate	1 (2.3%)	0 (0%)	2 (8.3%)	0 (0%)	2 (6.7%)
Formate	5 (12%)	3 (12%)	1 (4.2%)	2 (20%)	1 (3.3%)

Supplementary Table 4. Frequency of the subjects with fecal organic acids below detection limits (Study 1).

Data represents the proportions of the subjects in whom respective organic acids were detected. IBD patients were classified by endoscopic assessment.

Supplementary Table 5

	Total	Left	Rectal	p value
Site of disease	8.42±10.0	8.28±8.65	10.2±11.4	0.89 (ANOVA)

	Treated	Untreated	p value
Immunosuppressant	5.73±8.06	9.48±9.87	0.26 (Student's t test)
Prodrug of 5-ASA	8.21±8.89	12.44±14.96	0.35 (Student's t test)
PPI	10.83±9.62	8.27±9.60	0.52 (Student's t test)
Steroid	4.96±10.49	9.25±9.37	0.28 (Student's t test)
Probiotics	8.39±10.12	10.51±5.89	0.71 (Student's t test)

Supplementary Table 5. Effects of lesion site and drug treatment on fecal *n*-butyrate levels in UC patients (Study 1).

Data represents the mean $\pm$ SD of fecal *n*-butyrate levels (μmol/g) and the *p* value of UC patients with different lesion sites or drug treatments.

Supplementary Table 6

	Small Intestine	Colon	Both	p value
Site of disease	8.42±10.0	8.28±8.65	10.2±11.4	0.62 (Kruskal-Wallis)
	Treated	Untreated	p value	
Anti-TNF	5.30±4.84	5.11±4.52	0.90 (Student's t test)	
Immunosuppressant	6.04±5.08	4.82±4.47	0.45 (Student's t test)	
Prodrug of 5-ASA	5.26±4.52	4.98±5.76	0.90 (Student's t test)	
PPI	2.80±1.11	5.41±4.77	0.52 (Student's t test)	
Probiotics	5.70±5.20	4.22±3.17	0.35 (Student's t test)	

Supplementary Table 6. Effects of lesion site and drug treatment on fecal *n*-butyrate levels in CD patients (Study 1).

Data represents the mean $\pm$ SD of fecal *n*-butyrate levels (μmol/g) and the *p* value of CD patients with different lesion sites or drug treatments.

Supplementary Table 7

n-Butyrate

Bacterial genera	rho	FDR	Abundance in healthy subjects (%)
Haemophilus	0.55	0.000028	0.18
Faecalibacterium	0.53	0.000029	11.81
Eubacterium	0.51	0.000056	7.62
Roseburia	0.45	0.0010	0.79
Coprobacter	0.42	0.0031	0.03
Anaerostipes	0.39	0.0066	1.79
Eggerthella	0.35	0.022	0.33
Turicibacter	0.34	0.029	0.05
Parasutterella	0.34	0.029	0.39
Dorea	0.33	0.029	0.63
Ruminococcus	0.32	0.041	4.16
Gemmiger	0.32	0.041	2.67

Acetate

Bacterial genera	rho	FDR	Abundance in healthy subjects (%)
Proteus	0.46	0.0022	0.0017
Coprobacter	0.44	0.0022	0.03
Haemophilus	0.44	0.0022	0.18

n-Valerate

Bacterial genera	rho	FDR	Abundance in healthy subjects (%)
Faecalitalea	0.39	0.042	0.026

i-Butyrate

Bacterial genera	rho	FDR	Abundance in healthy subjects (%)
Bacillus	0.39	0.049	0.0078

Supplementary Table 7. Summary of bacterial genera associated with fecal organic acid levels (Study 1).

Data represent the Spearman's correlation coefficients, *p* values with Benjamini-Hochberg correction (FDR), and average bacterial abundance of healthy subjects (%). Bacteria abundant (more than 1 %) in the healthy subjects are shown in bold.

Supplementary Table 8

n-Butyrate

Bacterial species	rho	FDR	Abundance in healthy subjects (%)
Haemophilus parainfluenzae	0.55	0.000037	0.18
Eubacterium ventriosum	0.54	0.000037	0.60
Faecalibacterium prausnitzii	0.53	0.000044	11.64
Ruminococcus obeum	0.48	0.00054	0.58
Eubacterium rectale	0.48	0.00056	2.38
Faecalibacterium sp.	0.47	0.00060	0.08
Eubacterium ramulus	0.46	0.00084	0.29
Eubacterium hallii	0.43	0.0023	2.04
Anaerostipes hadrus	0.42	0.0029	0.48
Roseburia inulinivorans	0.42	0.0030	0.21
Coprobacter fastidioåsus	0.42	0.0032	0.03
Blautia glucerasea	0.39	0.0067	0.25
Anaerostipes sp.	0.39	0.0067	1.28
Roseburia intestinalis	0.39	0.0067	0.43
Roseburia faecis	0.37	0.014	0.04
Haemophilus pittmaniae	0.36	0.017	0.01
Eggerthella lenta	0.35	0.020	0.33
Phascolarctobacterium sp.	0.35	0.020	0.25
Ruminococcus gauvreauii	0.33	0.027	0.01
Clostridium xylanolyticum	0.34	0.027	0.11
Parasutterella excrementihominis	0.34	0.027	0.39
Ruminococcus faecis	0.34	0.027	0.89
Turicibacter sanguinis	0.34	0.027	0.05
Clostridium disporicum	0.33	0.028	0.05
Blautia schinkii	0.32	0.033	0.19
Ruminococcus bromii	0.31	0.043	2.12
Blautia wexlerae	0.31	0.045	3.16
Bacteroides vulgatus	0.31	0.049	4.05

Acetate

Bacterial species	rho	FDR	Abundance in healthy subjects (%)
Coprobacter fastidiosus	0.44	0.0089	0.030
Harmophilus parainfluenzae	0.43	0.0089	0.17

n-Valerate

Bacterial species	rho	FDR	Abundance in healthy subjects (%)
Ruminococcus gauvreauii	0.52	0.00035	0.013
Eubacterium cylindroides	0.39	0.048	0.026

Supplementary Table 8. Summary of bacterial species associated with fecal organic acid levels (Study 1).
Data represent the Spearman's correlation coefficients, *p* values with Benjamini-Hochberg correction (FDR), and average bacterial abundance of healthy subjects (%). Bacteria abundant (more than 1 %) in the healthy subjects are shown in bold.

Supplementary Table 9

O-glycan components	Healthy	UC		CD		p value
		Active	Remission	Active	Remission	
Sulfate	0.48±0.17	0.46±0.22	0.44±0.19	0.56±0.20	0.43±0.18	0.72 (ANOVA)
Sialic acid	0.18±0.14	0.14±0.09	0.21±0.17	0.24±0.10	0.24±0.17	0.16 (Kruskal-Wallis)
NeuAc	0.17±0.13	0.14±0.09	0.21±0.17	0.24±0.10	0.23±0.17	0.15 (ANOVA)
NeuGc	0.007±0.017	0.007±0.014	0.005±0.010	0.003±0.014	0.010±0.064	0.56 (Kruskal-Wallis)

Supplementary Table 9. Association between IBD and stool mucin *O*-glycan component ratio (Study 1). Data represent the mean ± SD of the ratio of each mucin *O*-glycan component per mucin *O*-glycan (nmol/nmol) and the *p* values of the healthy subjects and IBD patients classified by endoscopic assessment.

Supplementary Table 10

Disease	Detection ratio	*p* value
Healthy	8/38 (21%)	-
UC	17/38 (45%)	0.0497
CD	7/25 (28%)	0.558

Supplementary Table 10. Association between IBD and fecal NeuGc detection frequency (Study 1).

Data represent the proportion of subjects in whom NeuGc was detected. Statistical tests were performed using Fisher's exact test by comparing with healthy subjects.

Supplementary Table 11

Nutrient	Healthy	UC	FDR
Molybdenum (µg)	116.7 ± 34.7	134.7 ± 37.7	0.21
Copper (mg)	0.88 ± 0.21	0.95 ± 0.22	0.97
Manganese (mg)	2.1 ± 0.6	2.2 ± 0.5	0.97
Alcohol (g)	12.6 ± 15.6	0.19 ± 0.28	0.97
Chromium (µg)	5.7 ± 1.4	5.8 ± 2.3	0.97
Iodine (µg)	325.3 ± 237.7	475.9 ± 426.1	0.97
Magnesium (mg)	206.5 ± 51.4	224.7 ± 69.6	0.97
Biotin (µg)	23 ± 7.8	27.1 ± 10.1	0.97
Carbohydrate (g)	226.3 ± 42.5	247.1 ± 74.4	0.97
Salt (g)	8.3 ± 3.2	9.5 ± 3.3	0.97
Vitamin_K (µg)	164.5 ± 76.9	185 ± 59.3	0.97
Sodium (mg)	3286.8 ± 1260.1	3763.3 ± 1298.8	0.97
Soluble_fiber (g)	2.7 ± 0.9	2.8 ± 0.8	0.97
Ash (g)	14 ± 4.7	15.4 ± 4.7	0.97
Insoluble_fiber (g)	8.2 ± 2.3	8.5 ± 2	0.97
Iron (mg)	6.3 ± 1.7	7 ± 2.6	0.97
Niacin (mg)	15.8 ± 3.1	12.4 ± 4.5	0.97
Total_fiber (g)	11.8 ± 3.3	12.8 ± 3.5	0.97
Vitamin_B2 (mg)	0.83 ± 0.41	1.0 ± 0.67	0.97
Potassium (mg)	1984.5 ± 522.3	2006.7 ± 534.6	0.97
Vitamin_D (µg)	4.4 ± 2.3	4.5 ± 2.5	0.97
Retinol activity equivalent (µgRAE)	367.1 ± 190.4	429.2 ± 190.8	0.97
n6_fatty_acid (g)	9.9 ± 1.8	9.2 ± 4.2	0.97
Water (g)	860.3 ± 277	856.2 ± 323.9	0.97
Polyunsaturated_fat (g)	11.7 ± 2.1	11 ± 4.7	0.97
Saturated_fat (g)	18.7 ± 4.9	17.3 ± 8.5	0.97
Vitamin_B12 (µg)	4.3 ± 2.4	4.2 ± 1.8	0.97
Zinc (mg)	7.2 ± 1	6.7 ± 1.9	0.97
Vitamin_B1 (mg)	1.1 ± 0.23	0.91 ± 0.37	0.97
beta_carotene (µg)	2127.7 ± 1541.3	2377.7 ± 812.8	0.97
Monounsaturated_fat (g)	22.3 ± 3.7	18.8 ± 9.6	0.97
Retinol (µg)	160.7 ± 110.1	197.1 ± 159.3	0.97
beta_carotene equivalent (µg)	2455.7 ± 1730.1	2753.3 ± 894.5	0.97
Vitamin_B6 (mg)	1.2 ± 0.3	1.0 ± 0.3	0.97
Niacin equivalent (mg)	27.2 ± 5	23 ± 7	0.97
n3_fatty_acid (g)	1.9 ± 0.5	1.8 ± 0.6	0.97
Fat (g)	60.7 ± 12	55.7 ± 25.5	0.97
Fatty_acid (g)	52.7 ± 10.1	47.1 ± 22.4	0.97
Calcium (mg)	407.8 ± 199.4	507.3 ± 260.2	0.97
Energy (g)	1814.7 ± 271.2	1731.2 ± 559.6	0.97
Folate (µg)	232.1 ± 73.3	257.4 ± 69.8	0.97
Phosphorus (mg)	865 ± 195.9	847.7 ± 250.2	0.97
alpha_tocopherol (mg)	6.5 ± 1.4	6.7 ± 2.7	0.97
Cholesterol (mg)	293 ± 109.9	289.7 ± 135.8	0.97
Pantothenic_acid (mg)	5.2 ± 1.1	5.0 ± 1.6	0.97
Protein (g)	63.2 ± 11.9	57.3 ± 16.8	0.98
Vitamin_C (mg)	69.5 ± 25.5	74 ± 18	0.98
Selenium (µg)	55.5 ± 15.7	50.6 ± 16.5	0.99

Supplementary Table 11. Summary of the nutrient intake of healthy subjects and UC patients (Study 2). Data represent the mean ± SD of the daily nutrient intake and p values with Benjamini-Hochberg correction (FDR).