SUPPORTING INFORMATION

Non-Targeted LC-MS^n Profiling of Compounds in Ileal Fluids that Decrease After Raspberry Intake Identifies Consistent Alterations in Bile Acid Composition

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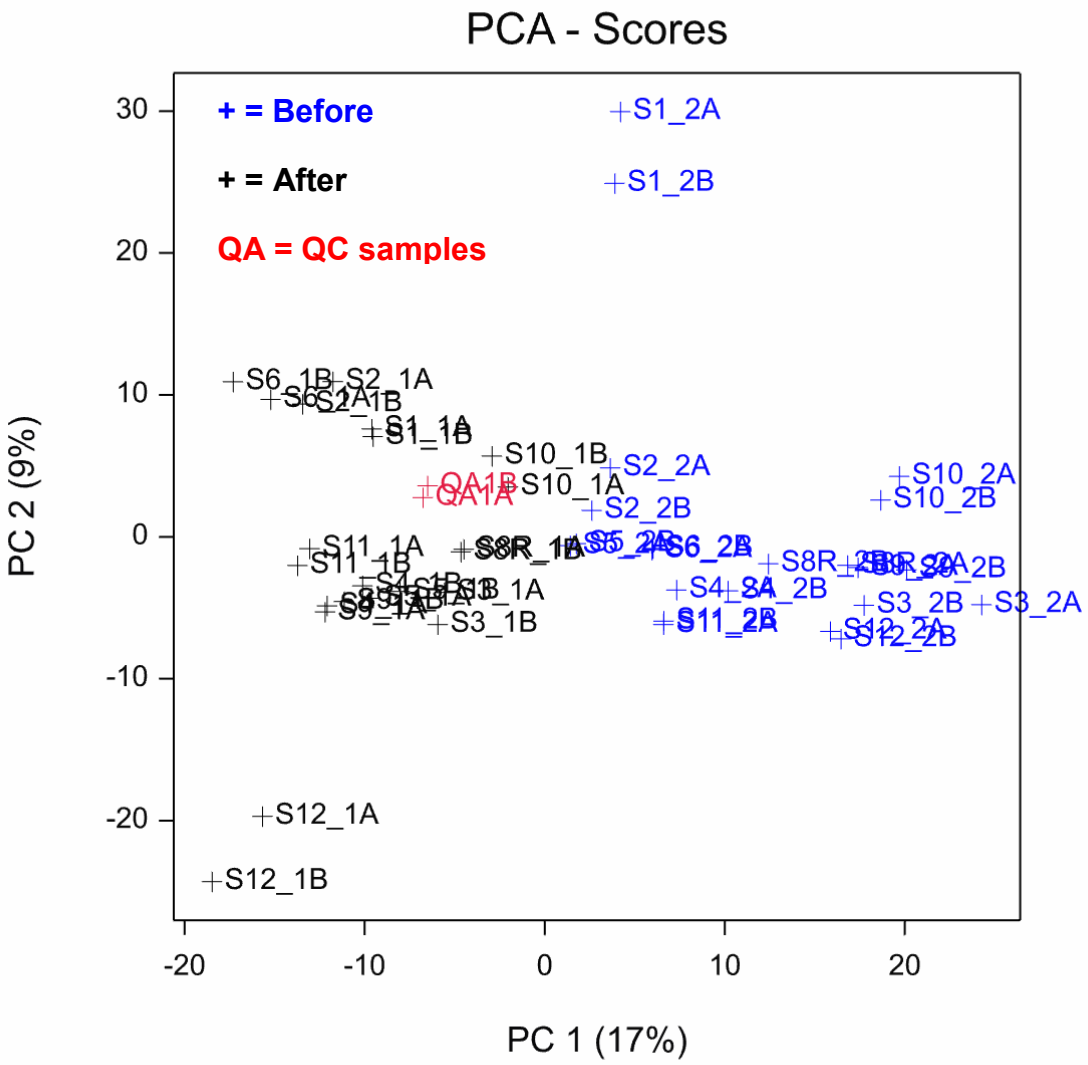

Figure S1A. Principal components analysis plot of MS data from ileal samples before and after raspberry supplementation.

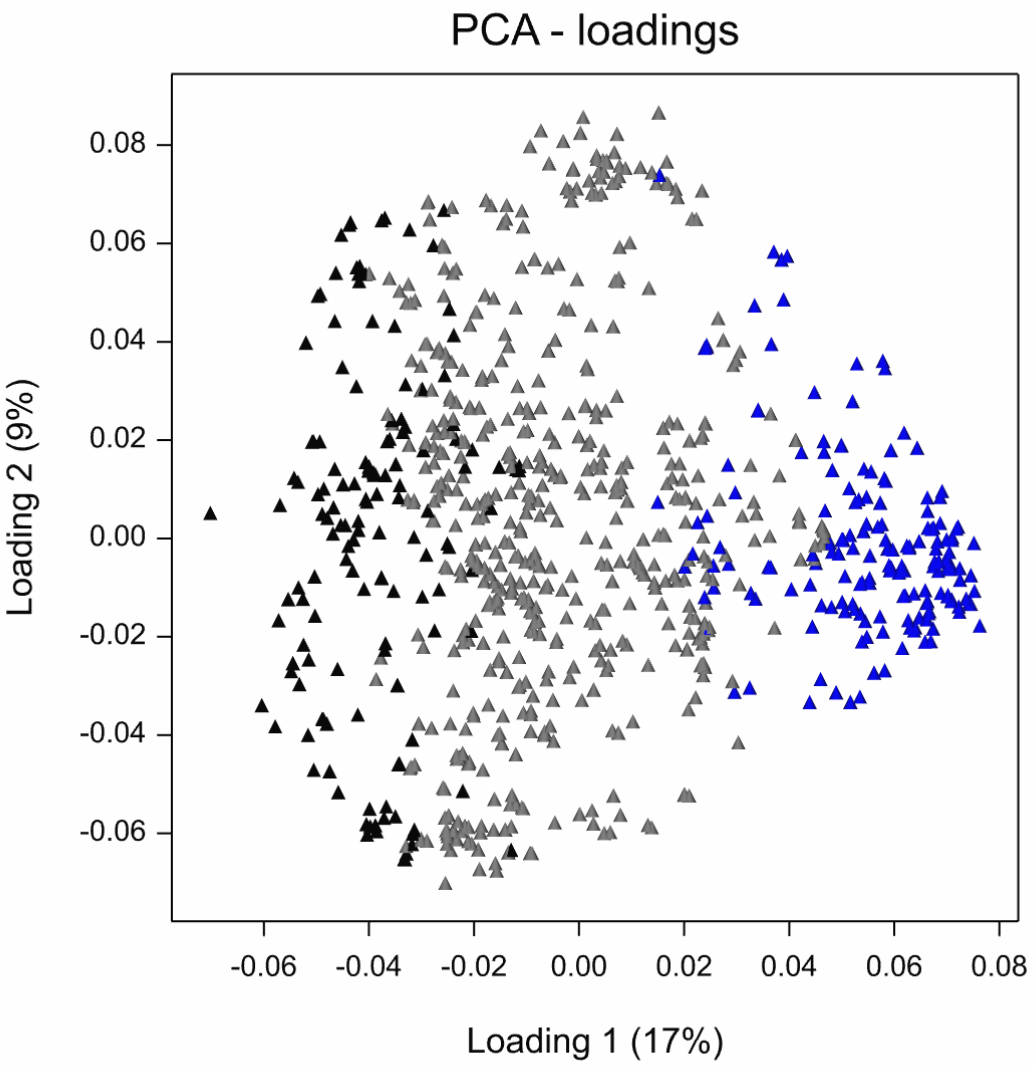

Figure S1B. Loadings plot from principle components analysis of MS data from ileal samples before and after raspberry supplementation. Black triangles are *m/z* signals that contribute most highly to the "after" signals, blue triangles contribute most to the "before" signals and grey triangles are the remainder.

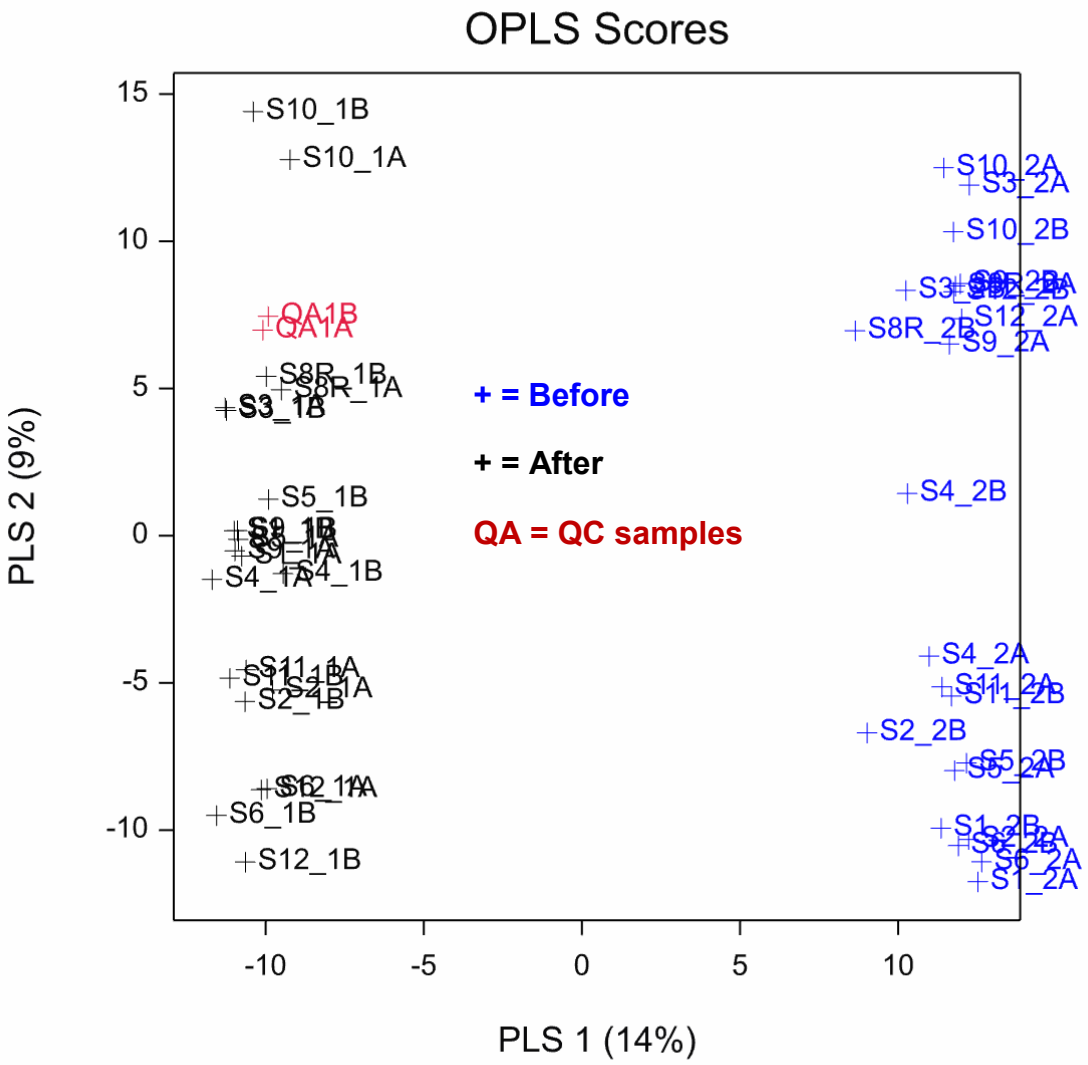

Figure S1C. OPLS-DA scores plot of MS data from ileal samples before and after raspberry supplementation. OPLS-DA analysis was applied to discriminate the before and after samples.

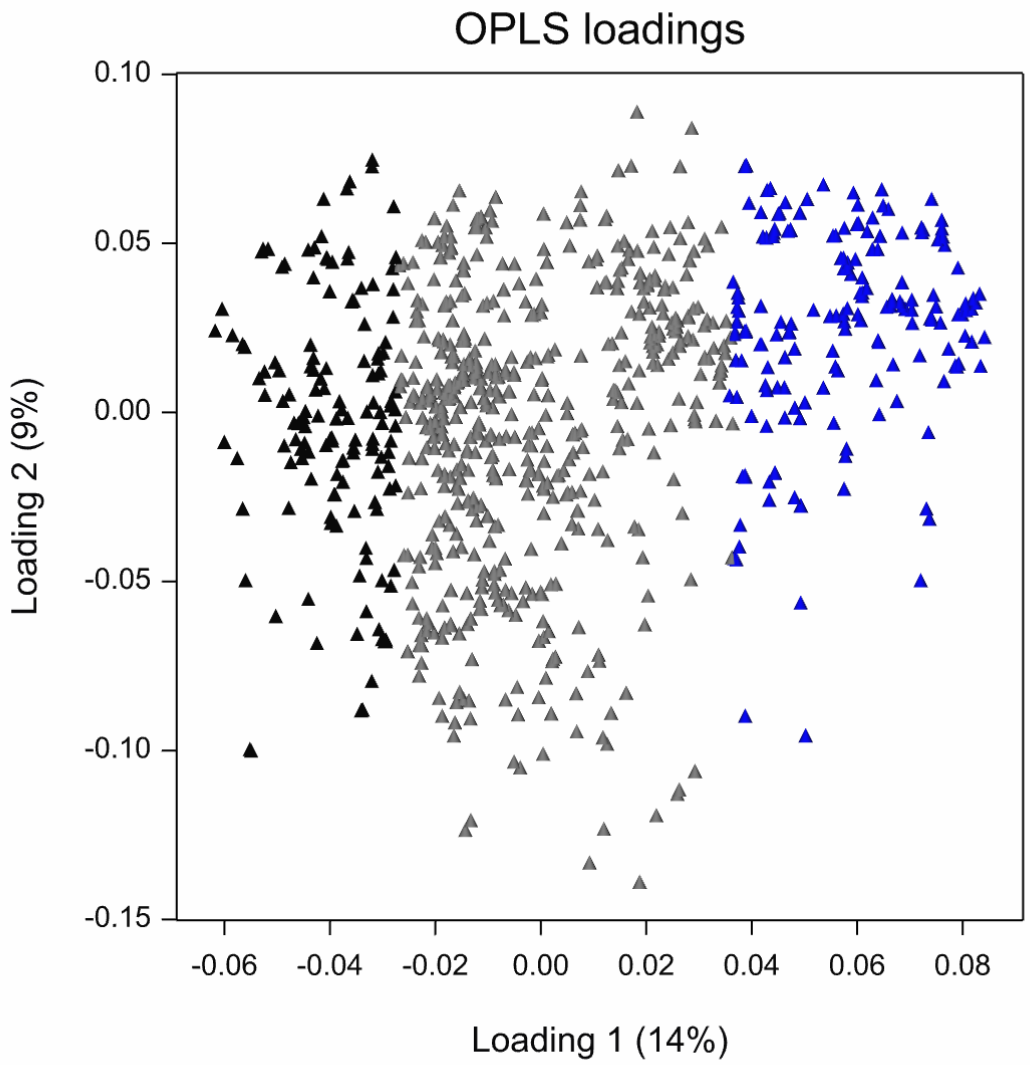

Figure S1D. Loadings plot from OPLS-DA analysis plot of MS data from ileal samples before and after raspberry supplementation. Black triangles are *m/z* signals that contribute most highly to the "after" signals, blue triangles contribute most to the "before" signals and grey triangles are the remainder.

Table S1. List of *m/z* Signals Associated with the "Before" Condition

The *m/z* values in bold were selected for further study. Isotopic or adduct variants were removed before the exclusion parameters were applied. Components had to be reduced in a minimum of 8 participants after raspberry intake. Some *m/z* values were deemed as "not real" as they lacked a characteristic peak shape. The lists obtained from the PCA and OPLS-DA loadings plots were effectively identical.

no.	*m/z* value	*Rt*	reason for exclusion
1	249.006	5.06	-
2	318.165	5.09	6d
3	326.123	5.32	-
4	246.006	6.17	3d
5	287.087	6.87	6d
6	165.041	6.92	7d
7	302.134	7.05	6d
8	225.087	7.08	-
9	218.102	7.26	6d
10	297.084	7.40	6d
11	117.055	8.04	-
12	204.98	8.27	-
13	149.027	8.47	-
14	161.081	8.94	5d
15	290.086	9.50	6d
16	253.118	9.58	-
17	158.081	10.28	6d
18	333.074	10.30	-

19	239.996	10.33	only present in 7
20	377.108	10.52	6d
21	181.05	10.58	-
22	363.106	10.58	7d
23	175.06	11.42	4d
24	189.076	11.63	7d
25	294.06	12.36	2d
26	399.084	12.58	-
27	178.05	12.78	-
28	567.273	12.89	-
29	227.055	12.96	7d
30	182.053	12.98	isotope?
31	181.05	12.98	correct?
32	363.106	12.99	charge variant?
33	364.11	12.99	5d
34	570.294	13.06	5d
35	569.29	13.06	5d
36	207.048	13.07	isotope
37	206.045	13.07	-
38	304.102	13.65	7d
39	259.071	13.76	-
40	239.996	14.03	-
41	177.076	14.16	6d

42	131.071	14.16	-
43	132.074	14.16	isotope
44	263.149	14.17	-
45	204.065	14.49	6d
46	192.066	14.62	-
47	305.068	14.81	6d
48	306.071	14.81	isotope of 305, 6d
49	333.026	14.88	4d
50	307.083	15.55	6d
51	363.118	15.62	-
52	330.201	15.64	-
53	190.05	15.75	3d
54	172.097	15.79	7d
55	273.086	16.13	4d
56	338.086	16.30	5d
57	184.097	16.50	-
58	225.112	16.68	5d
59	331.116	16.84	$[M-H]^{2-}$ ion of 165
60	165.055	16.85	-
61	166.058	16.85	isotope of 165
62	173.081	17.79	7d
63	320.151	18.87	5d
64	204.065	18.95	-

65	409.138	18.96	5d
66	236.091	19.02	7d
67	436.221	19.32	4d
68	320.076	20.68	4d
69	453.15	20.92	not real
70	455.165	21.31	6 d
71	359.042	21.42	-
72	187.096	21.89	5d
73	315.133	24.44	-
74	283.117	24.58	-
75	389.18	24.76	5d
76	343.174	24.78	5d
77	317.149	24.89	-
78	383.151	25.55	-
79	393.193	26.41	6d
80	469.278	26.49	-
81	267.106	26.64	7d
82	483.234	26.66	7d
83	366.099	26.75	5d
84	328.066	26.97	5d
85	346.221	27.14	only 7 down
86	453.283	27.15	not real
87	454.286	27.15	isotope

88	442.187	27.22	4d
89	407.278	27.28	non-formate adduct of 453
90	440.108	27.57	7 down
91	439.104	27.57	isotope
92	345.099	27.90	5d
93	469.278	28.32	5d
94	521.32	28.58	-
95	485.218	28.58	7d
96	535.336	28.63	6d
97	454.286	28.83	isotope
98	407.278	28.83	non-formate adduct of 453
99	453.283	28.85	-
100	345.226	28.90	5d
101	337.033	29.03	6d
102	439.279	29.04	5d
103	499.29	29.08	5d
104	536.32	29.42	not real
105	416.245	29.53	isotope
106	423.284	29.55	formate adduct of 373
107	373.167	29.56	6d
108	569.329	29.73	-
109	570.332	29.73	isotope
110	385.13	29.94	-

111	471.239	29.96	7d
112	488.238	30.03	isotope
113	487.234	30.03	-
114	420.24	30.16	5d
115	407.277	30.39	non-formate adduct
116	453.283	30.39	-
117	454.286	30.39	isotope of 453
118	816.566	30.41	isotope
119	815.562	30.41	charge variant 407
120	817.569	30.41	isotope
121	376.185	30.53	6d
122	375.182	30.53	isotope
123	451.267	30.61	isotope
124	452.271	30.61	6d
125	405.262	30.62	-
126	483.33	31.76	7d
127	553.334	32.12	6d
128	554.338	32.12	isotope
129	611.34	32.29	4d
130	451.268	32.31	isotope
131	814.551	32.33	charge variant 407
132	813.547	32.33	isotope of 814
133	407.277	32.36	non-formate adduct

134	454.286	32.48	isotope of 453
135	453.282	32.52	-
136	879.524	32.66	charge variant
137	880.527	32.67	isotope
138	472.242	32.78	6d
139	471.239	32.78	isotope
140	481.277	33.00	6d
141	285.205	33.21	5d
142	311.221	34.90	6d

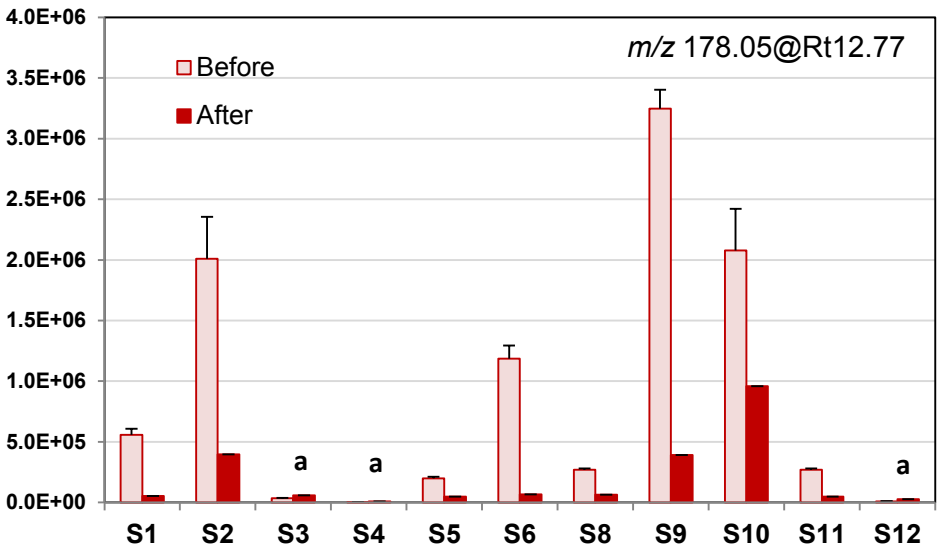

Figure S2A. Phenolic derivatives in ileal fluids - Hippuric acid.

Reduced in 8 of 11 participants, equivalent in 3 participants, a - after value is not significantly different from before value; $p = 0.01$.

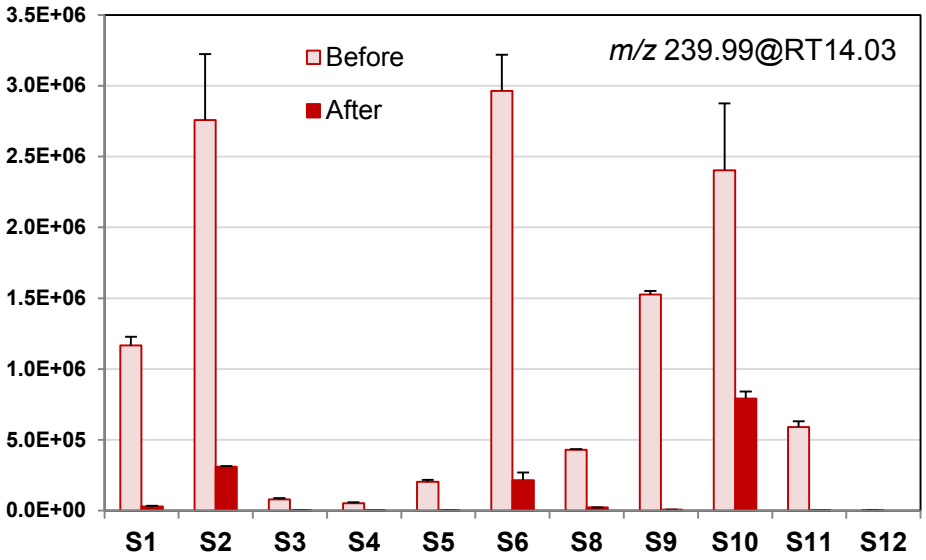

Figure S2B. Phenolic derivatives in ileal fluids - Indole carboxylic acid sulfate.

Reduced in all 11 participants; Factors range from x 2.2 (S12) to x 450 (S11).

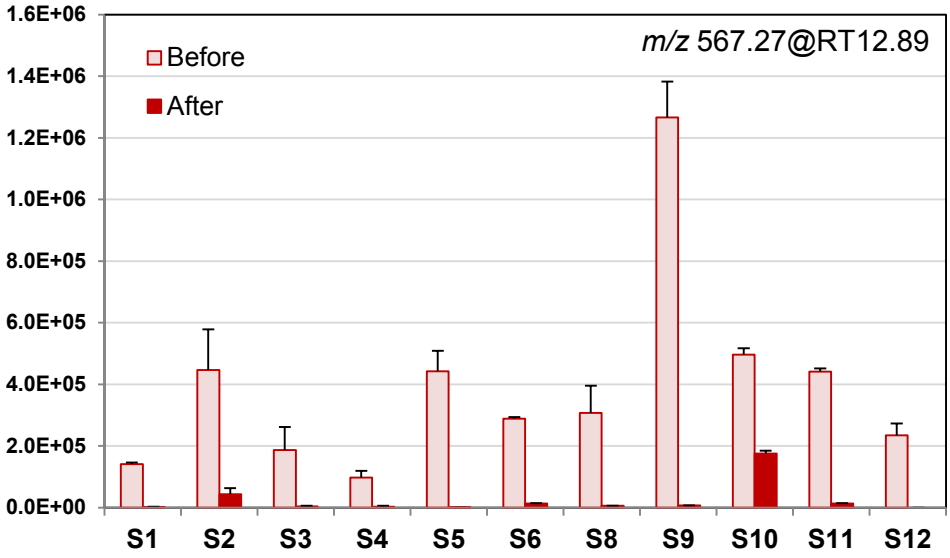

Figure S3. Leukotriene F4 content in ileal fluids**.**

Reduced in all 11 participants.