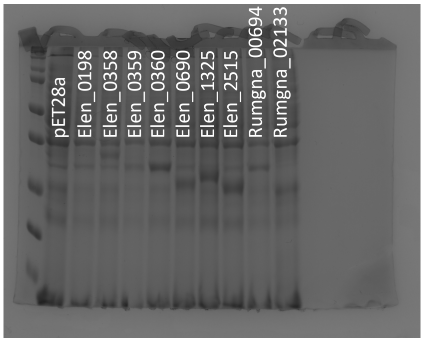
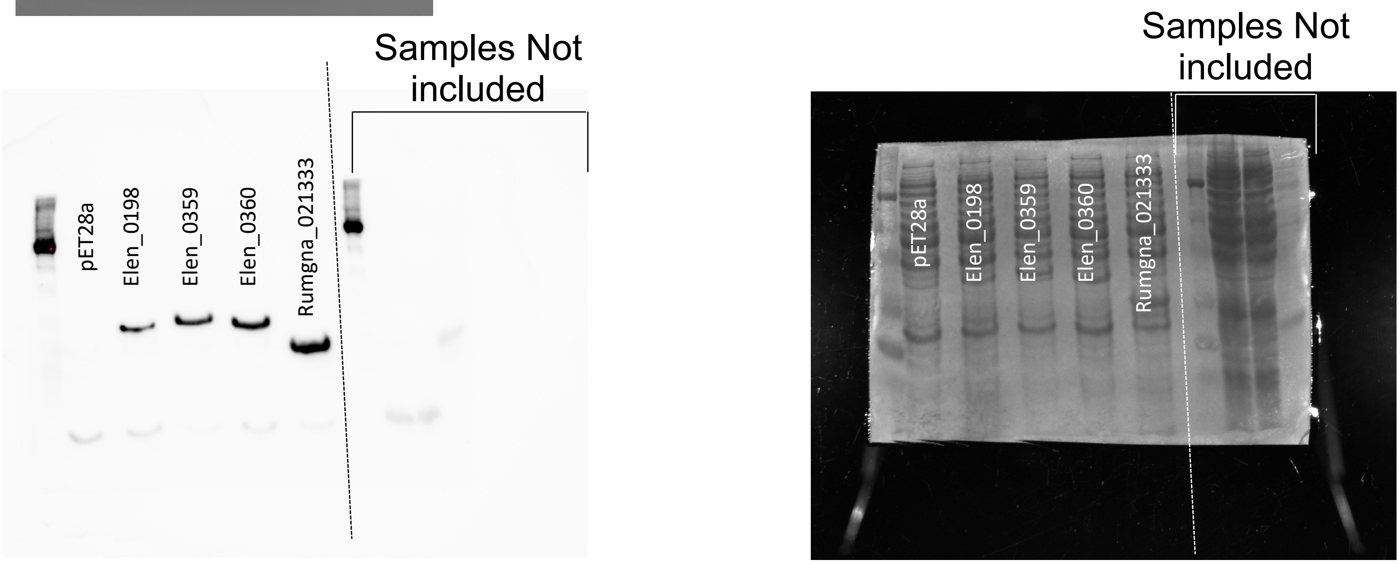
Supplementary Information
- Supplementary Figures

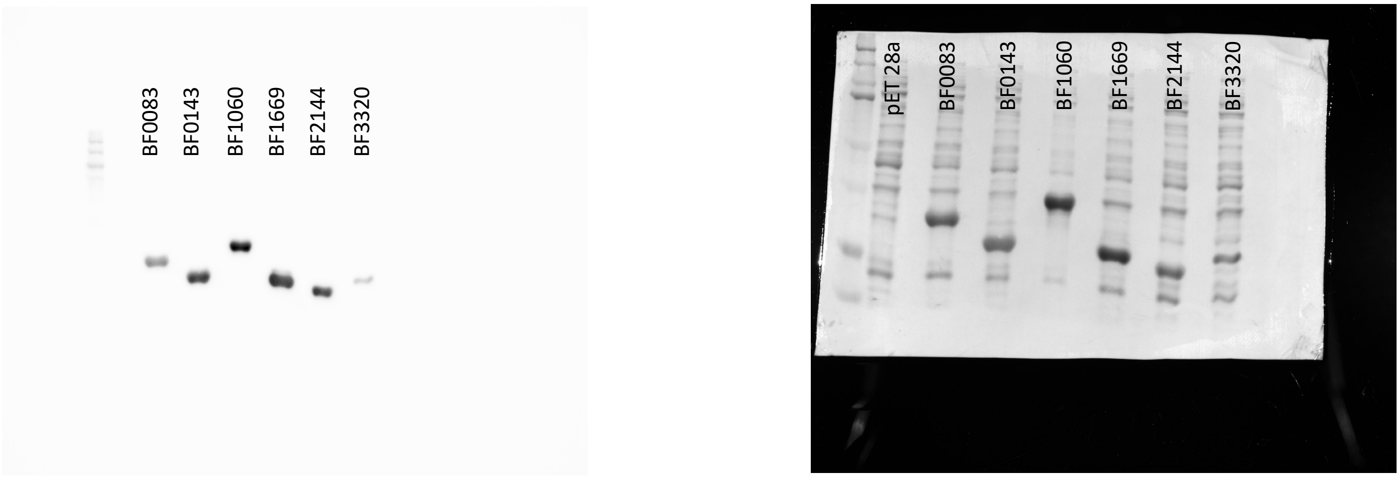
a



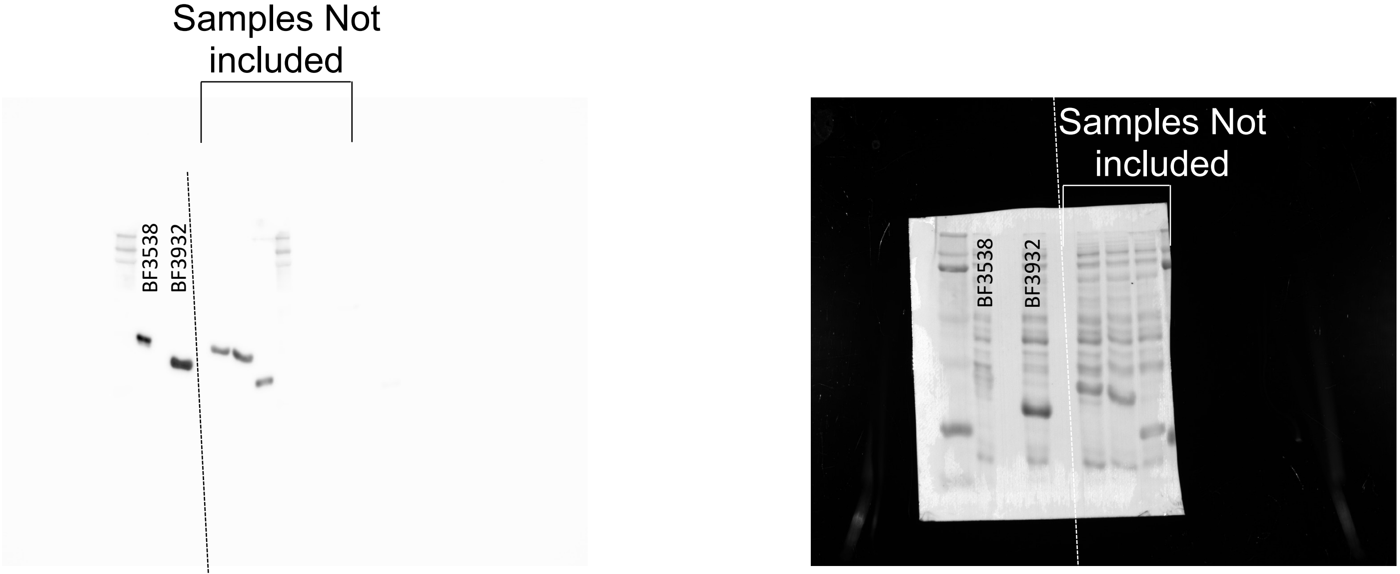
b

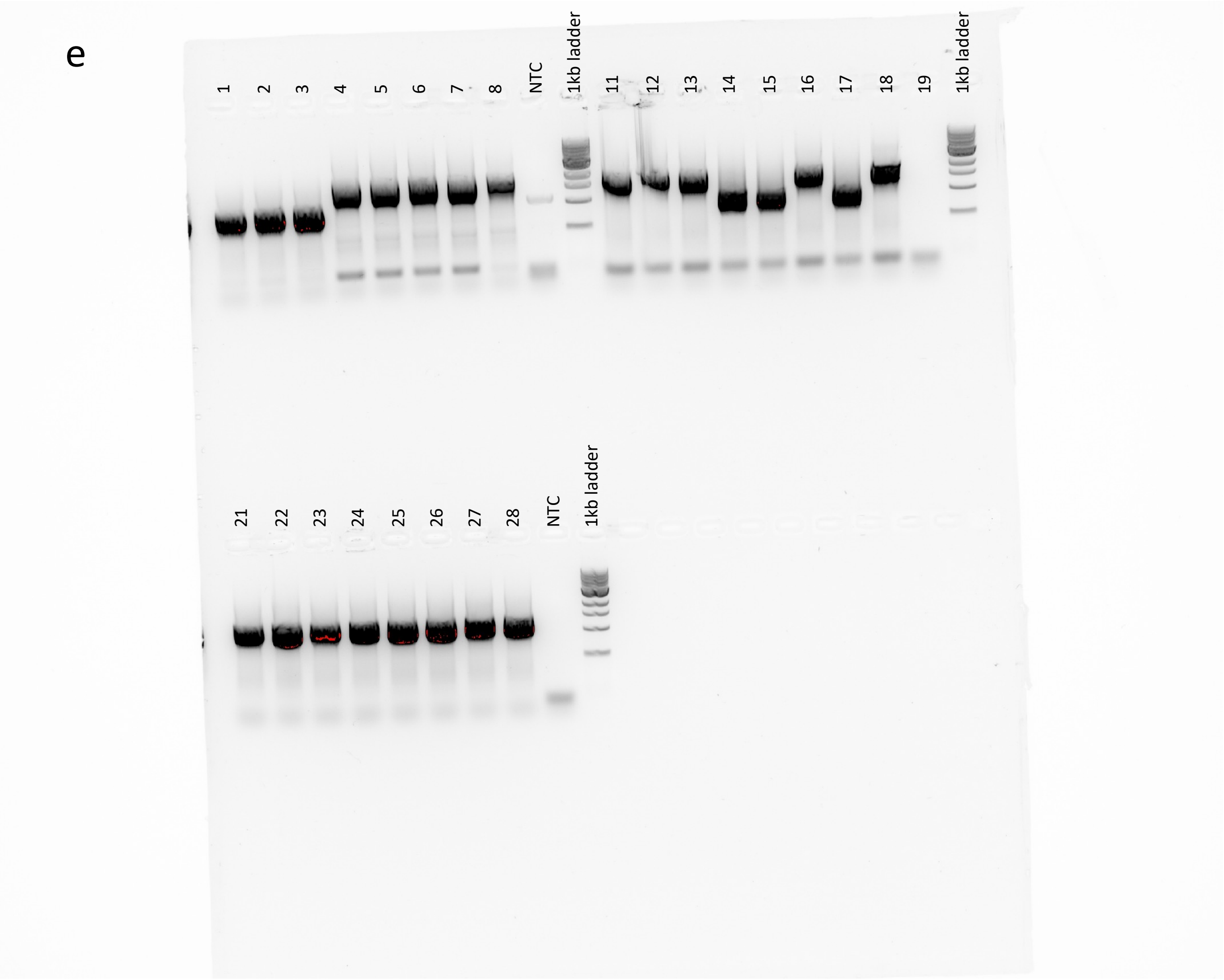


c



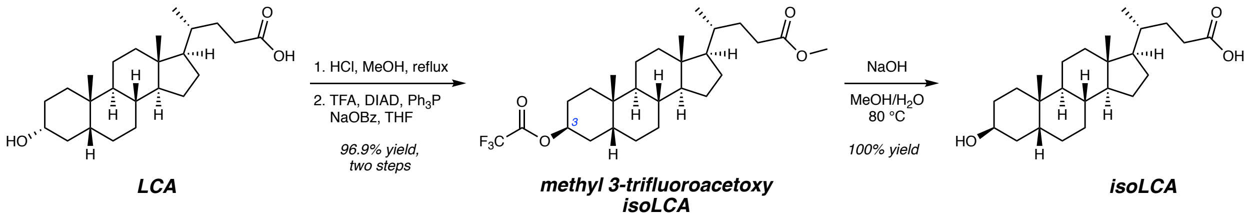
d





Supplementary Figure 1 | Gel and immunoblots raw images. a-d, source images for **Extended Data Fig. 4d-g**. **e**, source image for **Extended Data Fig. 4h**.

IsoLCA Synthesis Procedure.

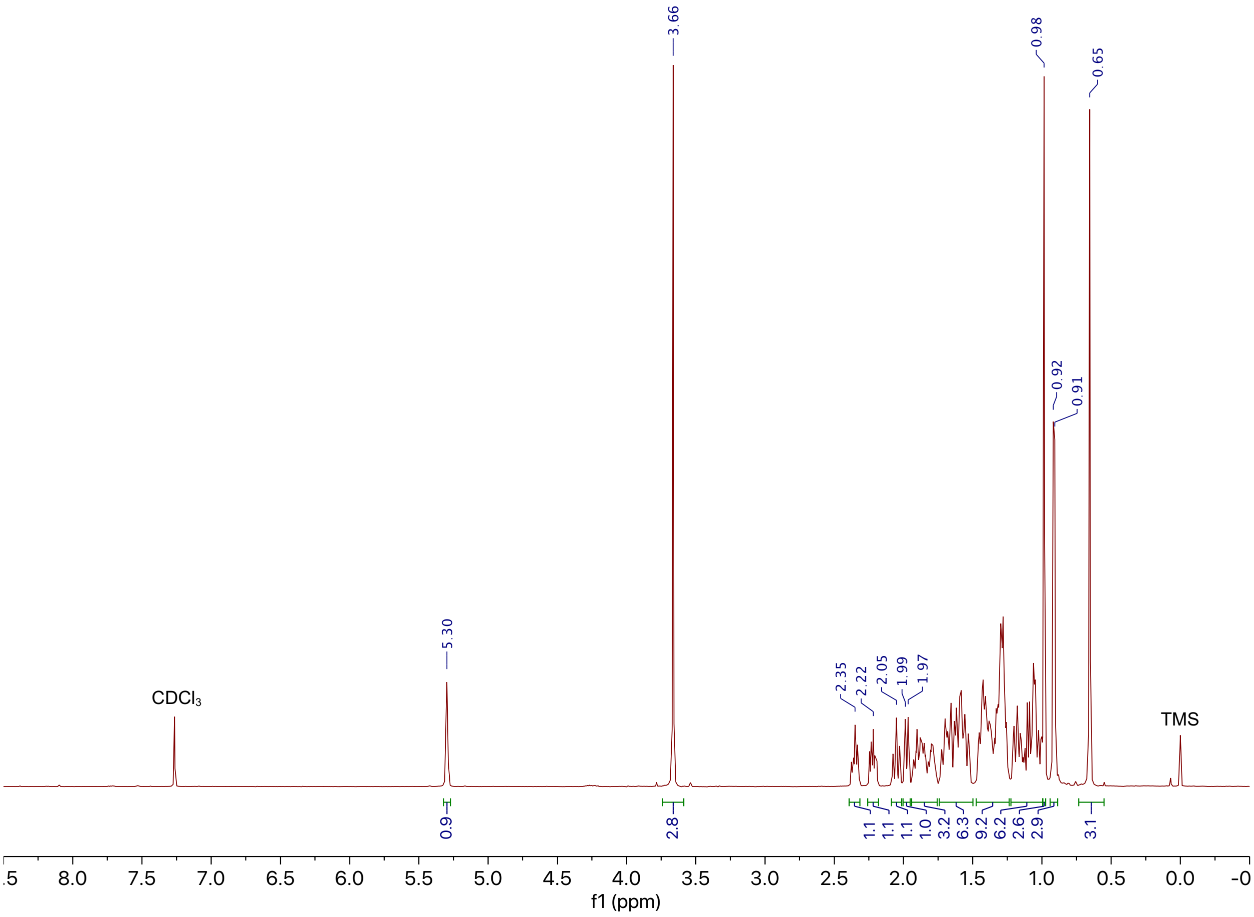


IsoLCA. Isolithocholic acid (isoLCA) was prepared from lithocholic acid (LCA) by carboxylic acid protection, then C3 alcohol inversion[56], followed by ester cleavage. Methanol (125 mL, 0.25 M) and HCl (622 µL of 1 M solution in methanol, 0.622 mmol, 0.02 equivalents) were added to a 500 mL round-bottom flask containing lithocholic acid (11.71 g, 31.10 mmol, 1 equivalent) and a stir bar. A reflux condenser was affixed to the flask and the contents were brought to reflux by immersion in a 90 °C oil bath with mixing. Upon completion by TLC analysis (1:1 hexanes/ethyl acetate; *p*-Anisaldehyde; overnight), the flask was cooled to room temperature and concentrated in vacuo. The resulting solid was further dried under high vacuum to afford methyl lithocholate as a free-flowing white solid (12.143 g, 31.087 mmol, 100% yield). $R_f = 0.35$ (2:1 hexanes/ethyl acetate; *p*-Anisaldehyde); mp = 130–132 °C (lit.[3] mp 130–132 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 3.66 (s, 3H), 3.62 (td, *J* = 10.9, 5.3 Hz, 1H), 2.35 (ddd, *J* = 15.4, 10.2, 5.1 Hz, 1H), 2.22 (ddd, *J* = 15.7, 9.9, 6.5 Hz, 1H), 1.95 (dt, *J* = 12.4, 3.2 Hz, 1H), 1.88–1.73 (m, 5H), 1.68–1.64 (m, 1H), 1.59–1.55 (m, 1H), 1.53–1.49 (m, 1H), 1.43–1.19 (m, 12H), 1.16–1.03 (m, 5H), 0.97 (td, *J* = 14.2, 3.4 Hz, 1H), 0.92 (s, 3H), 0.91 (d, *J* = 6.5 Hz, 3H), 0.64 (s, 3H); HRMS (DART+) *m/z*: $[M + NH_4]^+$ calculated for $C_{25}H_{46}O_3N$ 408.3478, found 408.3468; $[\alpha]_D^{21.3}$ +30.62 (*c* 1.07, CH_2Cl_2). All other compound data are consistent with reported values[57,58].

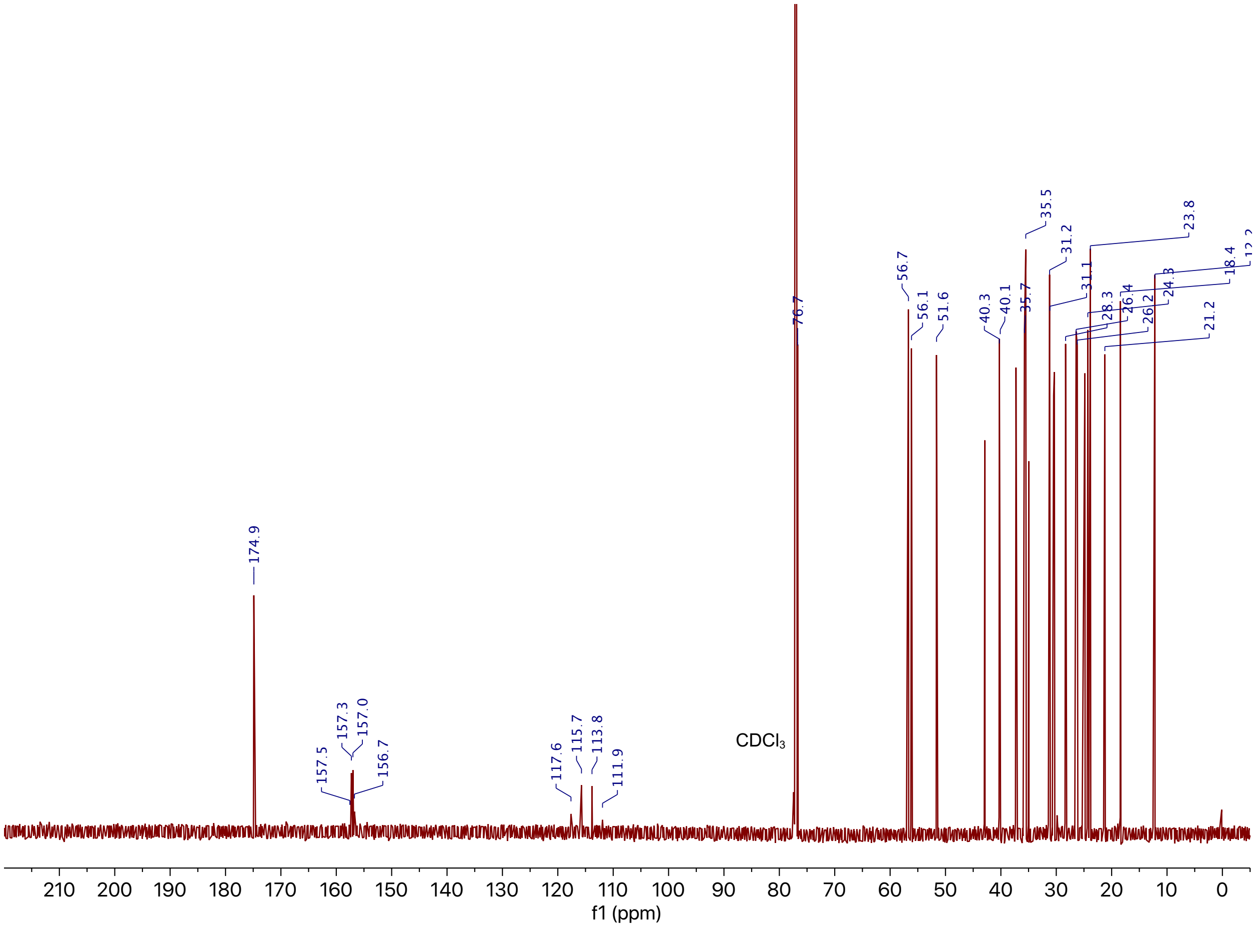
Tetrahydrofuran (105 mL, 0.3 M) was added to a flame-dried 500 mL round-bottom flask charged with methyl lithocholate (12.332 g, 31.571 mmol, 1 equivalent) and a stir bar under argon. To this colorless solution was added diisopropyl azodicarboxylate (DIAD: 6.84 mL, 34.73 mmol, 1.1 equivalents) and trifluoroacetic acid (TFA: 2.66 mL, 34.73 mmol, 1.1 equivalents), and the flask was placed in a room temperature water bath (T = 21 °C). Addition of triphenylphosphine (Ph_3P: 9.108 g, 34.73 mmol, 1.1 equivalents) to this bright orange solution resulted in a rapid color fading. Sodium benzoate (NaOBz: 5.005 g, 34.73 mmol, 1.1 equivalents) was then added and the white suspension was thoroughly mixed at room temperature. Upon completion by TLC analysis (2:1 hexanes/ethyl acetate; *p*-Anisaldehyde; ca. 4 h), hexanes (65 mL) were added. After mixing for at least 15 min, the reaction was filtered through a medium porosity Buchner funnel and the cloudy filtrate was concentrated in vacuo to yield an off-white solid. This crude solid (comprised of desired product, Ph_3PO, and reduced DIAD) was dissolved in CH_2Cl_2 (ca. 150 mL), dry-loaded onto a mixture of Celite (15 g) and SiO_2 (90 g), and purified by flash chromatography (6 x 21 cm SiO_2, 10% ethyl acetate in hexanes; collect fractions in 125–250 mL Erlenmeyer flasks) to afford methyl 3-trifluoroacetoxy isolithocholate as a white crystalline solid (14.885 g, 30.589 mmol, 96.9% yield). R_f = 0.37 (9:1 hexanes/ethyl acetate; *p*-Anisaldehyde); mp 142–145 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 5.30 (br s, 1H), 3.66 (s, 3H), 2.35 (ddd, *J* = 15.4, 10.2, 5.2 Hz, 1H), 2.22 (ddd, *J* = 15.8, 9.9, 6.5 Hz, 1H), 2.05 (ddd, *J* = 15.7, 13.5, 2.9 Hz, 1H), 1.99–1.96 (m, 1H), 1.93–1.77 (m, 3H), 1.73–1.53 (m, 6H), 1.46–1.26 (m, 9H), 1.21–1.00 (m, 6H), 0.98 (s, 3H), 0.91 (d, *J* = 6.5 Hz, 3H), 0.65 (s, 3H).; ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 174.9, 157.1 (q, *J* = 41.6 Hz), 114.8 (q, *J* = 286.2 Hz), 76.7, 56.7, 56.1, 51.6, 42.9, 40.3, 40.1, 37.3, 35.7, 35.5, 35.0, 31.2, 31.1, 30.5, 30.4, 28.3, 26.4, 26.2, 24.8, 24.3, 23.8, 21.2, 18.4, 12.2; ^{19}F NMR (376 MHz, $CDCl_3$): δ –75.4 (s); IR (ATR): 2973, 2929, 1777, 1737, 1435, 1213, 1185, 1152, 859 cm^{-1}; HRMS (DART+) *m/z*: $[M + NH_4]^+$ calculated for $C_{27}H_{45}O_4F_3N$ 504.3301, found 504.3289; $[\alpha]_D^{22.0}$ +15.95 (*c* 1.08, CH_2Cl_2). NMR spectra are shown in **Supplementary Fig. 2, 3** and **4**.

Methanol (146 mL), H_2O (29 mL; 5:1 methanol:H_2O, 0.1 M), and NaOH (4.24 g, 106 mmol, 3 equivalents) were added to a 1 L round-bottom flask charged with methyl 3-trifluoroacetoxy isoLCA (17.254 g, 35.312 mmol, 1 equivalent) and a stir bar. A reflux condenser was affixed to the flask, and the contents were placed under argon and warmed in an 80 °C oil bath with mixing. The suspension turned homogeneous over an hour. Upon reaction completion by TLC analysis (2:1 hexanes/EtOAc; *p*-Anisaldehyde; ca. 3 h), the flask was cooled to room temperature and methanol was removed in vacuo to yield a viscous slurry. H_2O (400 mL) was added to this slurry and the contents were sonicated, followed by acidification to pH < 3 with 1 M HCl (ca. 125 mL). The precipitate was sonicated for at least 10 min to ensure a free-flowing solid, then cooled in an ice bath and isolated via vacuum filtration. Washing and further drying of the filter cake (air, then 110 °C oven over night, then high vacuum) yielded isolithocholic acid as a powdery white solid (13.419 g, 35.634 mmol, 100% yield).

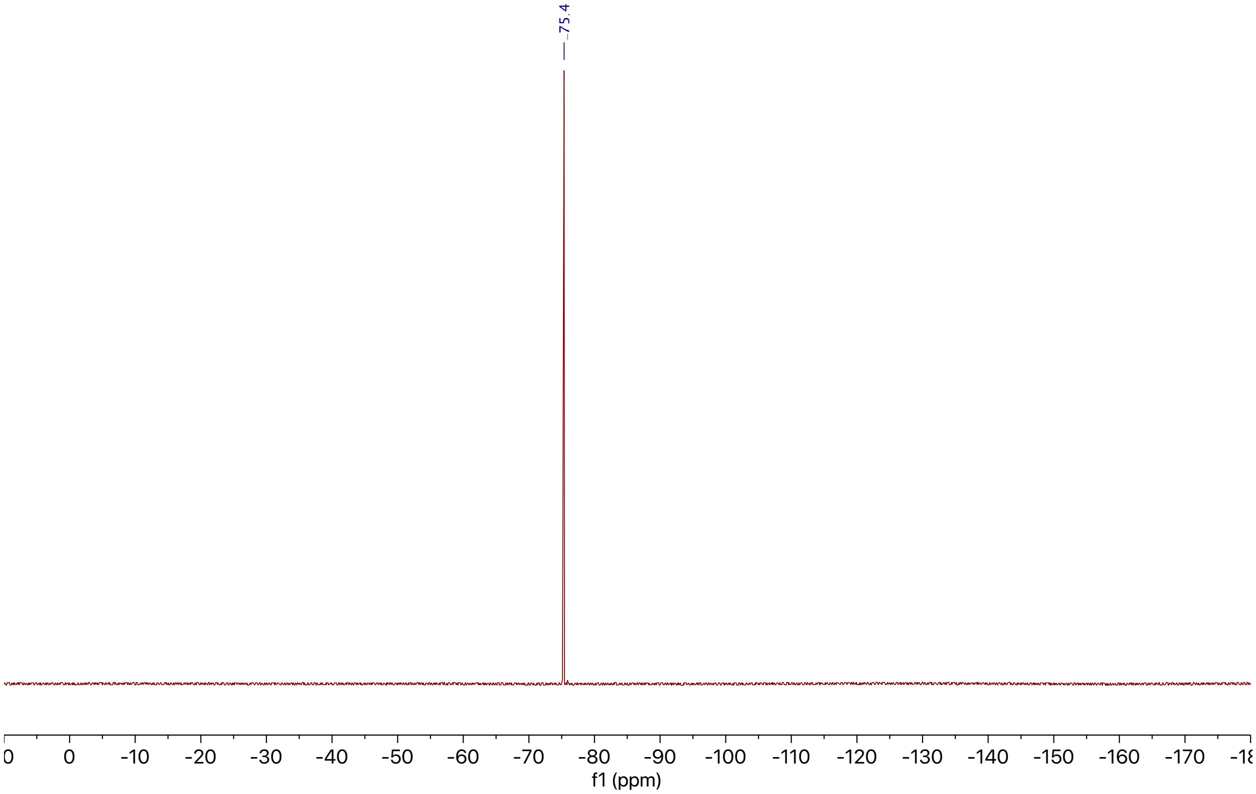
Characterization data[59]: R_f = 0.12 (1:1 hexanes/ethyl acetate; *p*-Anisaldehyde); mp 154–158 °C; ^{1}H NMR (600 MHz, CD_3OD): δ 4.03 (p, *J* = 2.7 Hz, 1H), 2.32 (ddd, *J* = 15.2, 9.8, 5.3 Hz, 1H), 2.19 (ddd, *J* = 15.7, 9.5, 6.9 Hz, 1H), 2.01 (dq, *J* = 13.8, 3.0 Hz, 2H), 1.97–1.85 (m, 2H), 1.79 (dddd, *J* = 13.1, 9.8, 6.9, 2.8 Hz, 1H), 1.77–1.72 (m, 1H), 1.60 (dtd, *J* = 10.9, 6.1, 5.5, 3.3 Hz, 1H), 1.56 (ddd, *J* = 14.2, 4.7, 2.5 Hz, 1H), 1.49–1.38 (m, 8H), 1.35–1.26 (m, 4H), 1.22–1.06 (m, 6H), 0.97 (s, 3H), 0.95 (d, J = 6.6 Hz, 3H), 0.69 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, CD_3OD): δ 178.2, 67.8, 58.0, 57.5, 43.9, 41.6, 41.1, 37.8, 37.1, 36.7, 36.2, 34.4, 32.3, 32.01, 31.0, 29.2, 28.5, 27.9, 27.4, 25.3, 24.4, 22.2, 18.8, 12.5; IR (ATR): 3232, 2922, 2864, 1710, 1442, 1217, 1038, 957 cm^{-1}; HRMS (DART–) *m/z*: $[M – H]^-$ calculated for $C_{24}H_{39}O_3$ 375.2899, found 375.2908; $[\alpha]_D^{22.4}$ +26.3 (*c* 0.805, CH_3OH). NMR spectra are shown in **Supplementary Fig. 5** and **6**.



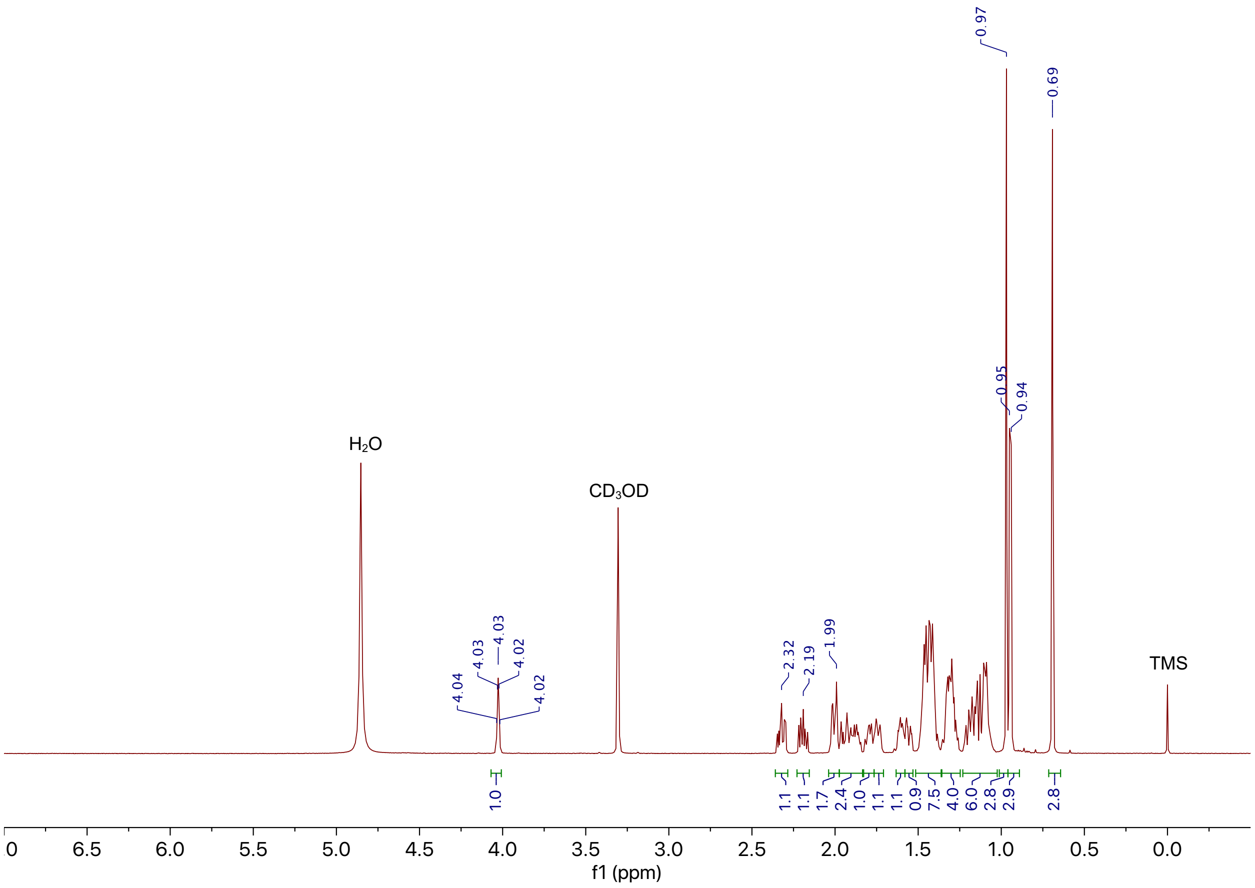
Supplementary Figure 2 | ^{1}H NMR spectrum (600 MHz, CDCl3) of methyl 3-trifluoroacetoxy isolithocholate. The compound data and spectrum of methyl 3-trifluoroacetoxy isolithocholate are representative of at least six synthesis experiments.



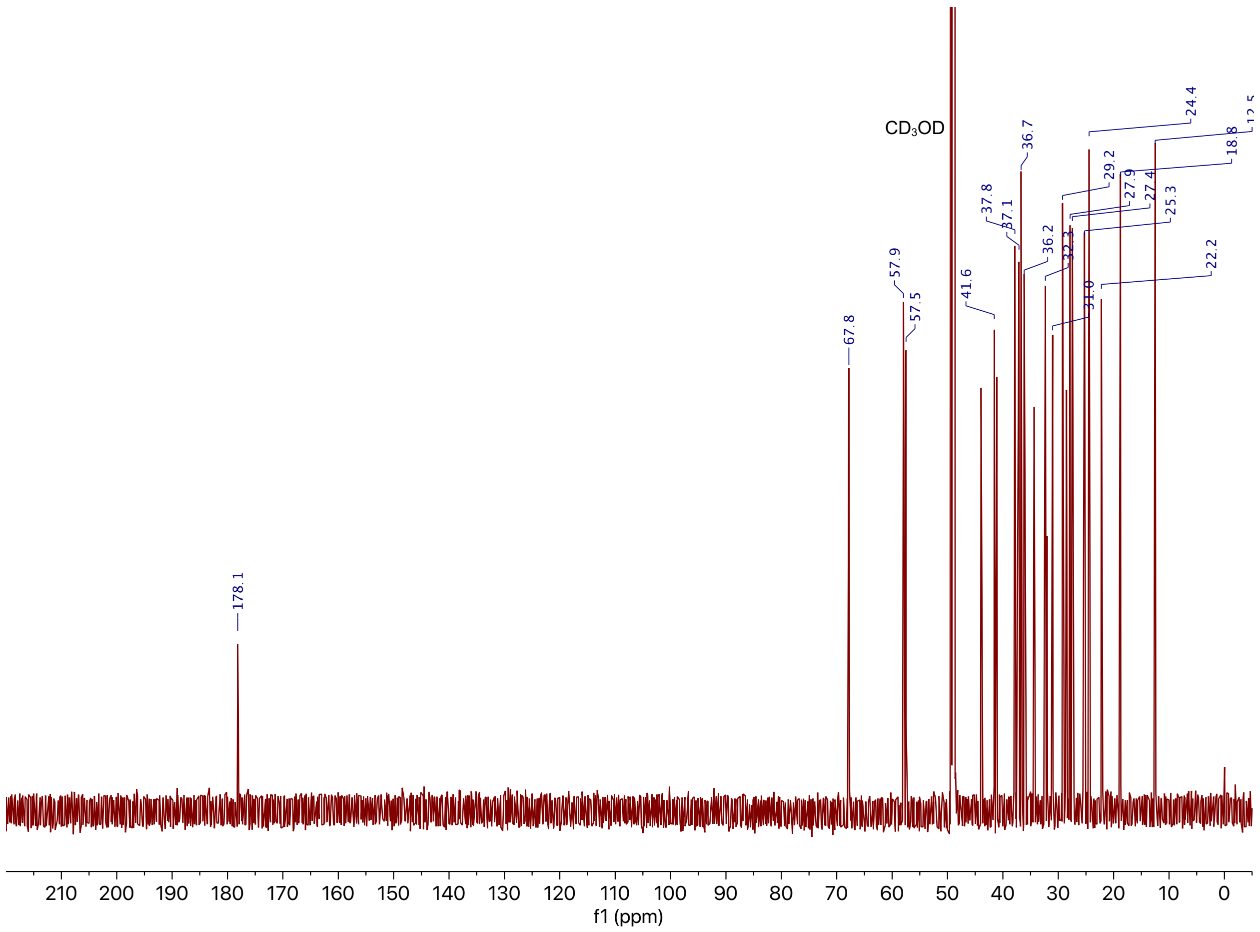
Supplementary Figure 3 | ^{13}C{^{1}H} NMR spectrum (151 MHz, CDCl3) of methyl 3-trifluoroacetoxy isolithocholate. The compound data and spectrum of methyl 3-trifluoroacetoxy isolithocholate are representative of at least six synthesis experiments.



Supplementary Figure 4 | ^{19}F NMR spectrum (376 MHz, CDCl3) of methyl 3-trifluoroacetoxy isolithocholate. The compound data and spectrum of methyl 3-trifluoroacetoxy isolithocholate are representative of at least six synthesis experiments.

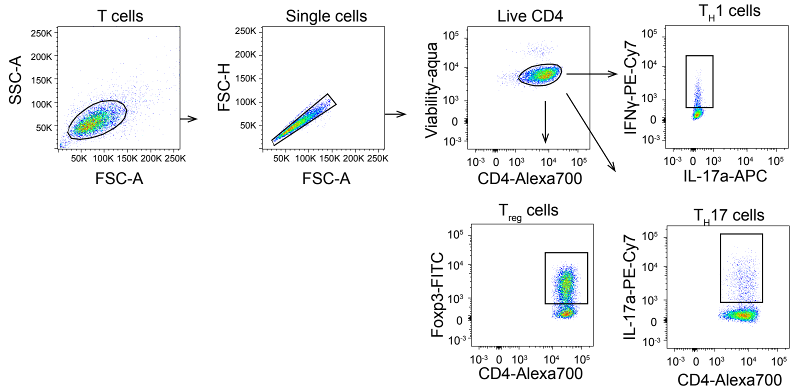


Supplementary Figure 5 | ^{1}H NMR spectrum (600 MHz, CD3OD) of isolithocholic acid.
The compound data and spectrum of isoLCA are representative of four synthesis experiments.

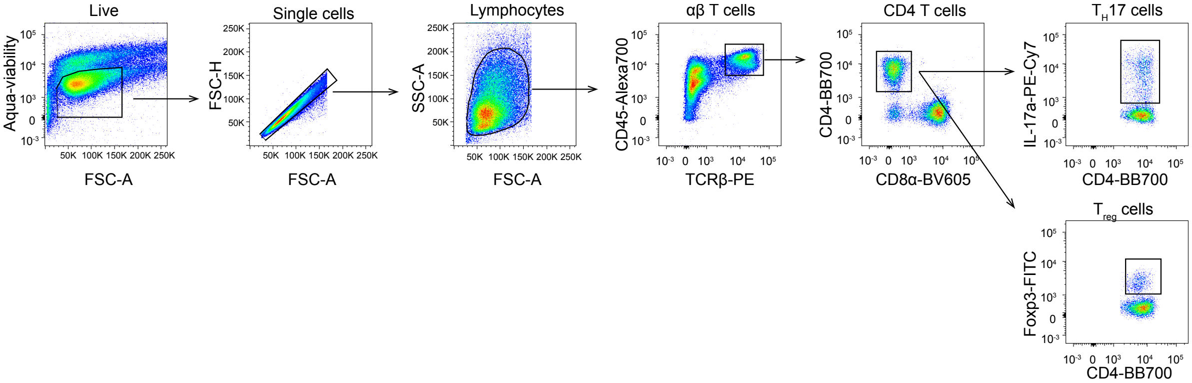


Supplementary Figure 6 | $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, CD3OD) of isolithocholic acid. The compound data and spectrum of isoLCA are representative of four synthesis experiments.

a In vitro T cell gating stragety

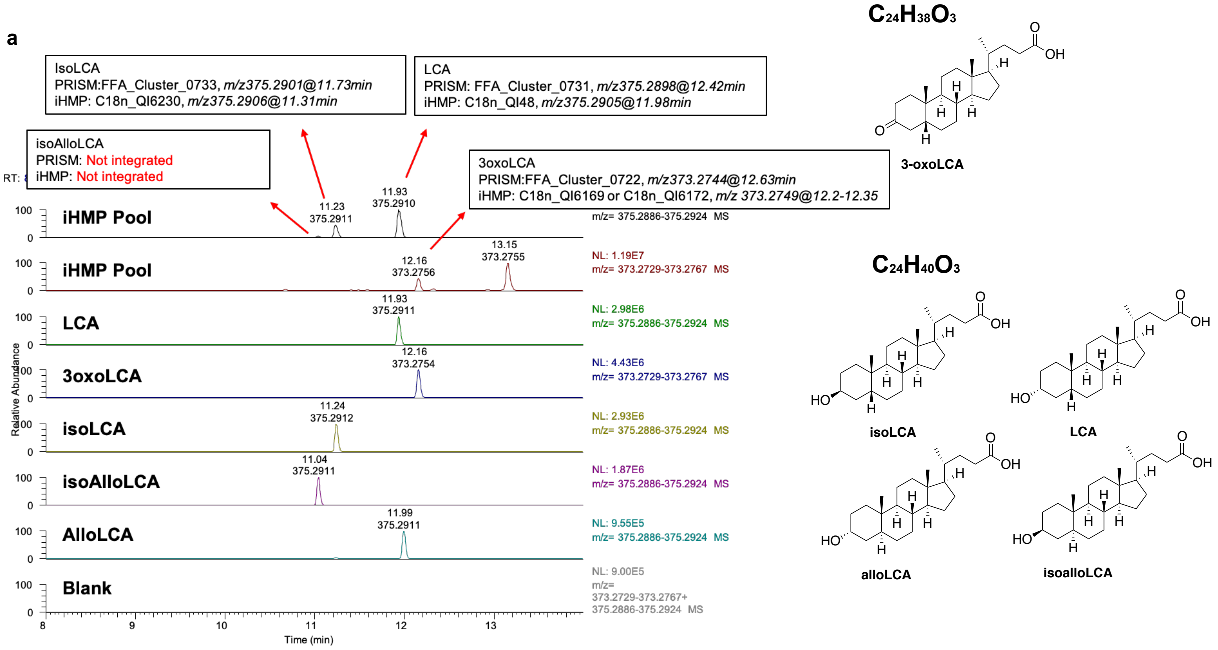


b In vivo lamina propria T cell gating stragety

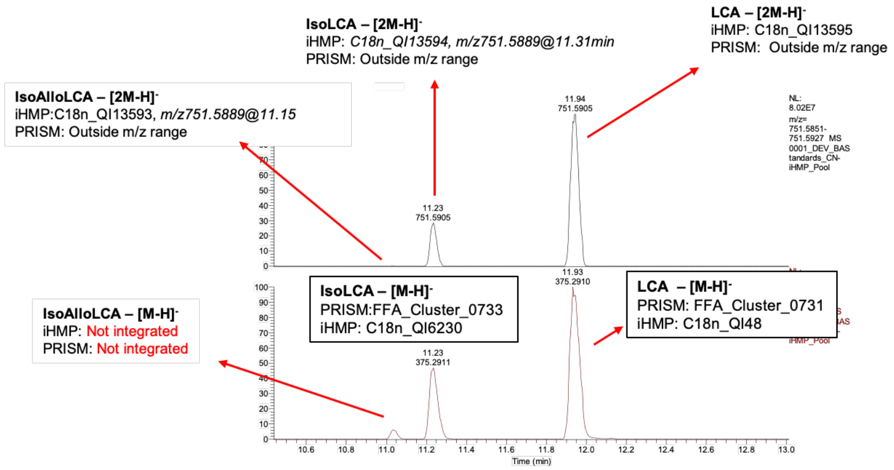


Supplementary Figure 7 | Gating strategy for the flow cytometric analyses of in vitro cultured T cells (**a**) and in vivo derived cells from the lamina propria (**b**).

a

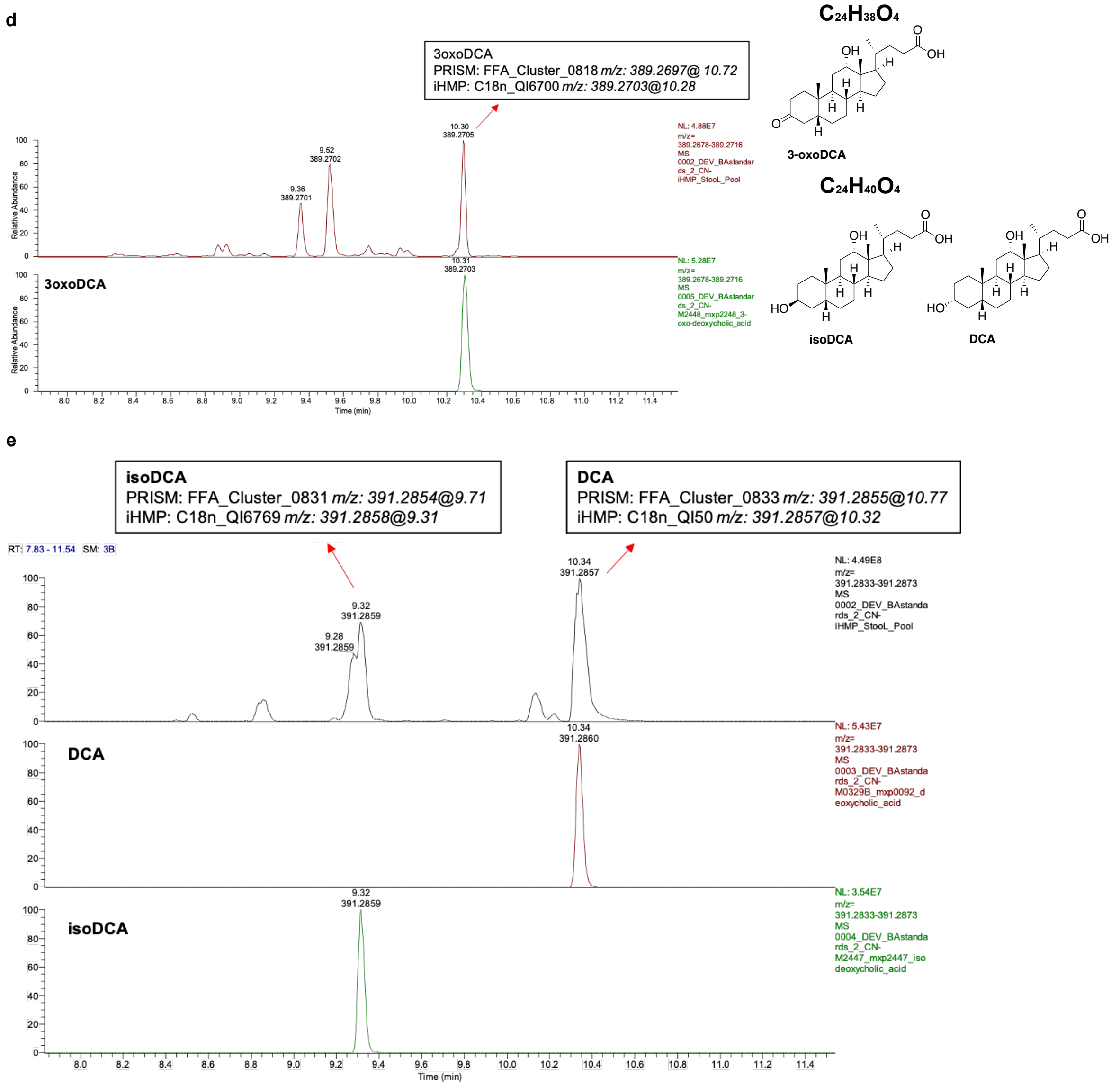


b



c

Compound	m/z	RT	iHMP Feature	iHMP m/z	iHMP RT (min)	Adduct	PRISM Feature	PRISM m/z	PRISM RT (min)	Adduct
3-oxoLCA	373.2748	12.16	C18n_QI6169 or C18n_QI6172	373.2749	12.2-12.35	[M-H]-	FFA_Cluster_0722	373.274	12.63	[M-H]-
LCA	375.2905	11.93	C18n_QI48	375.2905	11.98	[M-H]-	FFA_Cluster_0731	375.29	12.42	[M-H]-
			C18n_QI13595	751.5891	11.98	[2M-H]-				
isoLCA	375.2905	11.24	C18n_QI6230	375.2906	11.31	[M-H]-	FFA_Cluster_0733	375.29	11.73	[M-H]-
			C18n_QI13594	751.5889	11.31	[2M-H]-				
isoalloLCA	375.2905	11.04	C18n_QI13593	751.5889	11.15	[2M-H]-				
alloLCA	375.2905	11.99	Can't tell from LCA				Can't tell from LCA			



Supplementary Figure 8 | Identification of modified LCAs and DCAs mapped to PRISM and HMP2 metabolome database. **a**, EIC of molecules of interest run alongside the HMP2 stool pool. **b**, Additional features (adducts and fragments) were detected for the LCA isomers. Among the strongest signals was one corresponding to the formation of a dimer (2M-H). Unlike the M-H, this dimer m/z was integrated for all compounds in the non-targeted data in HMP2. This feature is not reported in PRISM because the method used had a narrower m/z range. **c**, Summary table of modified LCAs in PRISM and HMP2. **d**, EIC of 3-oxoDCA run alongside the HMP2 stool pool. **e**, EIC of isoDCA and DCA run alongside the HMP2 stool pool.

- Supplementary Tables

Supplementary Table 1 | Key Reagent Table

Chemicals		
DMSO	Sigma	D8418
Ethyl acetate	Sigma	319902
HCl	Sigma	258148
Methanol	EMD Millipore	MX0475
Ethanol	Sigma	E7023
PBS	Genesee Scientific	25-507
Vitamin K1-hemin	BD Biosciences	212354
Trace minerals	ATCC	MD-TMS
Trace vitamins	ATCC	MD-VS
FBS	Genesee Scientific	25-514
Cellobiose	Sigma	C7252
Maltose	Sigma	M5895
Fructose	Sigma	F0127
Arginine	Sigma	A5006
Yeast extract	Bacto	212750
Malt extract	Sigma	70146
Dextrose	Sigma	G5767
Phorbol 12-myristate 13-acetate (PMA)	Sigma	P1585
Ionomycin	Sigma	I3909
GolgiPlug	BD Biosciences	555029
Liberase TM	Sigma	5401127001
Dnase I (grade II, from bovine pancreas)	Sigma	10104159001
Bile acids		
LCA	Sigma	L6250
3-oxoLCA	Steraloids	C1750-000
IsoLCA	Steraloids	C1475-000
IsoalloLCA	Steraloids	C0700-000
AlloLCA	Steraloids	C0680-000
T-LCA	Steraloids	C1472-000
DCA	Sigma	D2510
3-oxoDCA	Steraloids	C1725-000
IsoDCA	Steraloids	C1165-000
CDCA	AstaTech	76487
TCA	Sigma	T4009
βMCA	Steraloids	C1895-000
GCA	Sigma	G2878
Antibodies		
For flow cytometry; specific folocs are indicated in the figures.		
Anti-IL-17a (eBio17B7)	eBioscience	25-7177-82
Anti-FoxP3 (FJK-16s)	eBioscience	11-5773-82
Anti-RORγt (B2D)	eBioscience	17-6981-82
Anti-IFNγ (XMG1.2)	eBioscience	48-7311-82
Anti-CD3ε (145-2C11)	eBioscience	48-0031-82

Supplementary Table 1 | Key Reagent Table (continued)

Anti-CD25 (PC61.5)	eBioscience	25-0251-82
Anti-CD62L (MEL-14)	eBioscience	11-0621-85
Anti-CD4 (RM4-5)	eBioscience	56-0042-82
Anti-CD45 (30-F11)	Biolegend	103128
Anti-CD8α (53-6.7)	Biolegend	100744
Anti-CD19 (6D5)	Biolegend	115540
Anti-CD44 (IM7)	Biolegend	103032
Anti-CD4 (RM4-5)	BD	566407
For in vitro T cell culture		
Anti-CD3ε (145-2C11)	eBioscience	16-0031-82
Anti-CD28 (37.51)	eBioscience	16-0281-82
Anti-hamster IgG (whole molecule) goat affinity-purified	MPBio	856984
For western blotting		
Anti-His-tag Antibody (rabbit polyclonal)	Cell Signaling	2365
Cytokines		
Human IL-2	PEPROTECH	200-02
Mouse IL-6	eBioscience	14-8061-62
Mouse IL-12	PEPROTECH	210-12
Human TGFβ1	PEPROTECH	100-21
Primers		
16s_ElentaF	CAGCAGGGAAGAAATTCGAC	
16s_ElentaR	TTGAGCCCTCGGATTAGAGA	
16s_BragilisF	TGTAACACGTGTGTAGCCCC	
16s_BragilisR	GGTTATGCTGAGGACTCTAG	
16s_RgnavusF	GGTAGTTGGTGGGGTAACGG	
16s_RgnavusR	TGTCTCAGTCCCAATGTGGC	
16s_CinnocuumF	CAGCTCGTGTCGTGAGATGT	
16s_CinnocuumR	CTCGCATGAGTCCCCAACTT	

Supplementary Table 2 | Human isolate screen metatables. Table fields in the 1-10 sheets named PLATE1 through PLATE11 indic-ate eleven 96-well plates containing 990 colonies from two patients' stool samples were collected (Methods). Assays were performed in replicate plates using either 100 μM LCA or 100 μM 3-oxoLCA as the substrate. Conversion rates in percentage for each well are shown in yellow gradient highlights for 3α-HSDH activity and green gradient highlights for 3β-HSDH activity. Table fields in the 12-13 sheets follow the similar format as the previous eleven sheets for the positive bacterial metabolizers verified in the bacterial culture tubes in triplicates. MS data was collected without specifying masses.

- PLATE1

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate1	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P1-A1	Collinsella aerofaciens	0.44604	0.00000	97.52560	0.04763
P1-A10	Bacteroides fragilis	0.02749	0.12314	23.64419	31.58931
P1-A11		0.04274	0.06440	0.00000	0.00000
P1-A12		0.09501	0.00000	0.08520	0.00000
P1-A2	Collinsella aerofaciens	0.02380	0.09519	34.13654	5.18806
P1-A3	Collinsella aerofaciens	0.33216	0.00000	97.35310	0.03396
P1-A4	Catenibacterium mitsuokai	0.03153	0.03378	0.02209	91.11984
P1-A5	Collinsella aerofaciens	0.14841	0.03544	98.09128	0.00000
P1-A6	Collinsella aerofaciens	0.25392	0.03681	97.84818	0.05627
P1-A7		0.00000	0.00000	0.12799	0.83481
P1-A8	Collinsella aerofaciens	0.21991	0.00000	83.22174	0.00000
P1-A9	Collinsella aerofaciens	0.12935	0.05605	35.99106	5.64579
P1-B1	Bacteroides cellulosilyticus	0.02744	0.00000	97.30672	0.06369
P1-B10	Streptococcus salivarius	0.43195	0.00000	5.09541	1.14501
P1-B11		0.02002	0.12977	0.00000	1.06125
P1-B12	Bacteroides dorei	0.06070	0.00000	1.43275	9.54963
P1-B2		0.03586	0.05186	0.04441	21.90368
P1-B3	Collinsella aerofaciens	0.04314	0.02988	97.75235	0.07245
P1-B4		0.03052	0.00000	0.04674	0.02771
P1-B5	Collinsella aerofaciens	0.19071	0.00000	98.24994	0.08661
P1-B6	Collinsella aerofaciens	0.18698	0.04394	98.22308	0.13030
P1-B7	Collinsella aerofaciens	0.05210	0.10616	33.89225	4.82254
P1-B8	Bacteroides cellulosilyticus/ intestinalis	0.02399	0.10406	0.00000	19.78247
P1-B9	Collinsella aerofaciens	0.00000	0.05178	33.02611	4.59280
P1-C1	Bacteroides vulgatus	0.11860	0.50134	94.94904	2.27888
P1-C10	Collinsella aerofaciens	0.09886	0.04715	33.83207	5.07079
P1-C11	Bacteroides vulgatus	0.00000	0.08015	2.67418	7.53473
P1-C12		0.12093	0.00000	0.01887	0.11314
P1-C2	Bacteroides cellulosilyticus	0.13438	0.07398	97.55771	0.00000
P1-C3	Bifidobacterium longum	1.05545	0.00000	11.21356	16.90184
P1-C4	Collinsella aerofaciens	0.03670	0.04099	1.06936	0.00000

Sequence Summary Report

P1-C5	Collinsella aerofaciens	0.11097	0.05688	33.57453	5.04727
P1-C6	Collinsella aerofaciens	0.13993	0.05684	33.98396	5.02675
P1-C7	Collinsella aerofaciens	0.02790	0.00000	33.84925	4.72375
P1-C8	Collinsella aerofaciens	0.08036	0.04408	97.56328	0.26278
P1-C9	Collinsella aerofaciens	0.15869	0.02868	82.28676	0.00000
P1-D1		0.11188	0.08829	0.22668	2.20661
P1-D10	Collinsella aerofaciens	0.07922	0.02980	32.73685	4.91519
P1-D11		0.00000	0.00000	0.00000	31.10003
P1-D12		0.08476	0.20323	0.00858	0.00000
P1-D2	Bacteroides uniformis	0.05365	0.03028	0.00000	28.13904
P1-D3	Collinsella aerofaciens	0.20849	0.00000	98.11412	0.00000
P1-D4	Bacteroides cellulosilyticus	0.02121	0.07653	0.00000	27.95430
P1-D5		0.01667	0.03098	0.08488	0.57821
P1-D6	Collinsella aerofaciens	0.02126	0.06600	97.97734	0.00000
P1-D7	Bacteroides cellulosilyticus	0.02476	0.07838	0.00000	28.68572
P1-D8	Parabacteroides merdae	0.02301	0.05161	0.00000	17.86859
P1-D9	Collinsella aerofaciens	0.03792	0.03596	6.92291	1.38880
P1-E1	Collinsella aerofaciens	0.04253	0.03403	36.19458	5.75837
P1-E10		0.02118	0.00000	0.01217	0.03165
P1-E11	Collinsella aerofaciens	0.34342	0.00000	99.39099	0.10886
P1-E12	Collinsella aerofaciens	0.27301	0.13269	99.88469	0.08919
P1-E2		0.00000	0.11259	0.00000	0.24271
P1-E3	Collinsella aerofaciens	0.01720	0.02635	99.77632	0.00000
P1-E4		0.02336	0.00000	0.01630	0.07094
P1-E5	Collinsella aerofaciens	0.17141	0.03486	91.61052	1.53582
P1-E6		0.00000	0.06590	0.48258	8.59895
P1-E7	Collinsella aerofaciens	0.15425	0.10111	99.57845	0.08853
P1-E8		0.04396	0.03345	0.00000	14.44001
P1-E9	Collinsella aerofaciens	0.05514	0.05776	31.01376	1.19468
P1-F1		0.03585	0.04717	0.31920	0.00000
P1-F10	Bacteroides uniformis	0.02609	0.09498	0.00000	21.57717
P1-F11	Collinsella aerofaciens	0.13779	0.00000	98.65641	0.09182
P1-F12	Collinsella aerofaciens	0.00000	0.16891	33.63692	3.40649
P1-F2	Bifidobacterium pseudocatenulatum	0.08834	0.00000	1.73747	24.01944
P1-F3	Bacteroides cellulosilyticus/ intestinalis	0.03397	0.03940	0.00000	27.15558
P1-F4		0.09185	0.02476	0.01002	0.09501
P1-F5		0.10864	0.02827	0.03360	0.33838

Sequence Summary Report

P1-F6	**Collinsella aerofaciens**	0.02059	0.00000	98.14397	0.05338
P1-F7	**Bacteroides cellulosilyticus/ intestinalis**	0.06908	0.03878	0.00000	26.56359
P1-F8		0.02955	0.03666	0.00000	26.05974
P1-F9	**Collinsella aerofaciens**	0.05560	0.07295	99.06028	0.11376
P1-G1	**Bacteroides cellulosilyticus**	0.11790	0.02846	98.06354	0.26742
P1-G10	**Collinsella aerofaciens**	0.21314	0.07202	99.33661	0.06390
P1-G11	**Collinsella aerofaciens**	0.19963	0.00000	99.73534	0.08072
P1-G12	**Bacteroides cellulosilyticus**	0.00000	0.00000	1.69723	1.08668
P1-G2	**Bacteroides rodentium**	0.00000	0.04228	0.00000	26.91233
P1-G3		0.06964	0.00000	0.04478	0.05463
P1-G4	**Collinsella aerofaciens**	0.09200	0.03686	99.37866	0.07556
P1-G5		0.04229	0.02481	0.00881	0.00000
P1-G6		0.04120	0.04161	0.02156	0.07405
P1-G7		0.02579	0.00000	0.55323	0.00000
P1-G8		0.13460	0.13430	0.13097	0.28562
P1-G9		0.13972	0.00000	0.01361	0.20632
P1-H1	**Bacteroides uniformis**	0.04826	0.00000	0.04207	24.57614
P1-H10	**Collinsella aerofaciens**	0.18343	0.05449	98.50101	0.07989
P1-H11		0.04622	0.00000	0.03578	0.04149
P1-H12	**Bacteroides sp. / Bacteroides cellulosilyticus**	0.09583	0.16651	0.00000	16.34538
P1-H2	**Bifidobacterium longum**	1.18248	0.00000	7.56200	12.50201
P1-H3	**Collinsella aerofaciens**	0.27860	0.00000	97.97894	0.00000
P1-H4		0.02079	0.07200	0.02956	0.02814
P1-H5	**Catenibacterium mitsuokai/ Catenibacterium sp.**	0.00000	0.12400	0.03176	85.95947
P1-H6		0.03371	0.04313	0.00920	0.02804
P1-H7		0.03182	0.00000	0.55225	1.71917
P1-H8	**Bifidobacterium longum**	0.87125	0.00000	10.65127	16.71063
P1-H9	**Collinsella aerofaciens**	0.14837	0.08053	99.50336	0.00000

- PLATE2

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate2	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P2-A1	Roseburia faecis	0.12362	0.25781	2.35201	0.85601
P2-A10		0.04265	0.15479	0.00000	0.00000
P2-A11		0.10892	0.55658	0.00000	0.09692
P2-A12		0.09747	0.15616	0.26136	39.61100
P2-A2	Lachnospira pectinoschiza	0.04369	0.00000	0.03024	72.25347
P2-A3		0.00000	0.00000	0.78339	0.62250
P2-A4	Murimonas intestini	0.10093	0.56119	3.95509	0.26514
P2-A5		0.11654	0.00000	0.00000	0.00000
P2-A6		0.24784	0.38302	0.00000	0.10160
P2-A7		0.11079	0.06529	0.10613	0.00000
P2-A8		0.22618	0.00000	0.00000	0.00000
P2-A9		0.07968	0.09809	0.04790	0.00000
P2-B1	Roseburia faecis	0.17984	0.00000	1.98632	1.22241
P2-B10		0.09287	0.12224	0.00000	0.00000
P2-B11		0.08035	0.16093	0.00000	0.00000
P2-B12		0.00000	0.00000	0.46000	0.82530
P2-B2		0.07889	0.08219	0.45197	1.67710
P2-B3		0.23817	0.05960	0.00000	0.00000
P2-B4		0.15764	0.10205	0.00000	0.00000
P2-B5		0.15129	0.09621	0.00000	0.00000
P2-B6	Clostridium citroniae	3.36551	5.59647	13.51704	1.48025
P2-B7		0.09889	0.07473	0.00000	6.70554
P2-B8		0.08234	0.07432	0.00000	0.00000
P2-B9		0.13331	0.11532	0.00000	0.00000
P2-C1		0.16696	0.09594	0.00000	0.00000
P2-C10		0.06820	0.08913	0.00000	0.41442
P2-C11		0.21407	0.07980	0.38246	0.00000
P2-C12		0.07224	0.13861	0.00000	0.00000
P2-C2		0.07709	0.00000	0.00000	0.00000
P2-C3		0.20313	0.10968	0.00000	0.00000
P2-C4		0.18868	0.00000	0.00000	0.00000

P2-C5	**Clostridium citroniae**	0.99419	2.06441	2.86249	9.24056
P2-C6		0.21486	0.00000	0.00000	0.00000
P2-C7		0.34449	0.21059	0.64004	0.00000
P2-C8		0.11697	0.00000	0.00000	0.00000
P2-C9		0.11503	0.18023	0.00000	0.00000
P2-D1		0.05209	0.00000	0.28362	0.00000
P2-D10		0.19091	0.21042	0.61587	0.00000
P2-D11		0.09181	0.10310	0.00000	0.00000
P2-D12	**Phocea massiliensis**	4.93739	0.08653	0.19928	0.00000
P2-D2		0.06144	0.10463	0.00000	0.00000
P2-D3		0.25152	0.00000	0.00000	0.00000
P2-D4		0.08885	0.07625	0.00000	0.00000
P2-D5		0.11977	0.10956	0.00000	0.00000
P2-D6		0.09073	0.06691	0.00000	0.00000
P2-D7		0.00000	0.05867	0.00000	19.10382
P2-D8		0.03079	0.00000	0.00000	0.00000
P2-D9		0.07003	0.06638	0.00000	0.00000
P2-E1		0.05233	0.00000	0.24556	0.23075
P2-E10		0.52698	0.00000	0.00000	0.00000
P2-E11		0.17586	0.07684	0.00000	0.00000
P2-E12		0.05184	0.20163	0.00000	0.00000
P2-E2		0.00000	0.09547	0.00000	0.00000
P2-E3		0.04098	0.00000	0.00000	0.00000
P2-E4		0.06008	0.06777	0.00000	0.00000
P2-E5		0.00000	0.11699	0.00000	0.00000
P2-E6		0.00000	0.13195	0.00000	0.00000
P2-E7		0.00000	0.11782	0.00000	0.00000
P2-E8	**Clostridium citroniae**	0.00000	0.25850	38.06156	16.32686
P2-E9	**Clostridium symbiosum**	0.11684	0.00000	1.02610	0.00000
P2-F1		0.06205	0.07664	0.20147	0.00000
P2-F10		0.07216	0.00000	0.00000	3.60249
P2-F11		0.08346	0.25721	0.00000	0.00000
P2-F12		0.07238	0.15120	0.00000	0.00000
P2-F2	**Lactobacillus rogosae**	0.00000	0.00000	0.00000	61.27788
P2-F3		0.05579	0.11597	0.00000	0.55976
P2-F4		0.17660	0.87449	0.55185	8.44035
P2-F5		0.23013	0.13340	0.50879	15.24047

Sequence Summary Report

P2-F6		0.09196	0.27258	0.56447	0.00000
P2-F7		0.18298	0.07514	0.00000	0.00000
P2-F8		0.06161	2.18083	0.00000	0.00000
P2-F9		0.08817	0.08383	0.00000	0.00000
P2-G1	**Lactobacillus rogosae**	0.20420	0.14005	0.10165	54.33423
P2-G10		0.20916	0.32300	0.00000	0.00000
P2-G11		0.17788	0.00000	0.40326	0.00000
P2-G12		0.07224	0.12949	0.00000	0.00000
P2-G2		0.14303	0.00000	0.52918	0.26432
P2-G3		0.22225	0.06524	0.20311	11.54807
P2-G4		0.08906	0.08379	0.34502	6.42764
P2-G5		0.11325	0.23689	0.00000	0.00000
P2-G6		0.26286	0.10425	0.00000	0.00000
P2-G7		0.78107	0.27826	0.00000	0.87031
P2-G8		0.49365	0.00000	0.00000	0.00000
P2-G9		0.12059	0.00000	0.00000	0.00000
P2-H1		0.00000	0.09745	0.07264	9.19698
P2-H10		0.13659	0.26695	0.00000	0.00000
P2-H11		0.07915	0.00000	0.00000	0.00000
P2-H12		0.30870	0.00000	0.09035	0.00000
P2-H2	**Roseburia faecis**	0.00000	0.24335	1.12360	0.00000
P2-H3		0.00000	0.00000	0.20900	0.31638
P2-H4		0.25369	0.08703	0.00000	0.00000
P2-H5		0.08617	0.10684	0.00000	0.00000
P2-H6		0.00000	0.18526	0.00000	0.00000
P2-H7		0.11217	0.00000	0.00000	0.00000
P2-H8		0.00000	0.07500	0.00000	0.00000
P2-H9		0.07229	0.12166	0.11989	0.00000

- PLATE3

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate3	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P3-A1		0.04669	0.04038	0.00000	0.00000
P3-A10		0.19176	0.28934	0.59043	0.00000
P3-A11		0.09648	0.10672	0.00000	0.00000
P3-A12		0.03841	0.06944	0.00000	0.00000
P3-A2		0.08071	0.06476	0.00000	0.00000
P3-A3		0.00000	0.05054	0.00000	0.00000
P3-A4		0.00000	0.04563	0.02744	0.00000
P3-A5		0.00000	0.00000	0.00000	0.00000
P3-A6		0.11399	0.05170	0.00000	0.00000
P3-A7		0.02592	0.00000	0.00000	0.00000
P3-A8		0.01965	0.02871	0.00000	0.00000
P3-A9		0.09683	0.00000	0.00000	0.00000
P3-B1		0.09850	0.07424	0.00000	0.00000
P3-B10		0.09136	0.00000	0.00000	0.00000
P3-B11		0.02729	0.03438	0.00000	0.00000
P3-B12		0.09084	0.06265	0.00000	0.00000
P3-B2		0.02591	0.13213	0.00000	0.00000
P3-B3		0.05501	0.00000	0.00000	0.00000
P3-B4		0.03076	0.03734	0.00000	0.00000
P3-B5		0.02277	0.00000	0.00000	0.00000
P3-B6		0.05139	0.00000	0.02944	0.00000
P3-B7		0.04378	0.05759	0.00000	0.00000
P3-B8		0.00000	0.10633	0.00000	0.00000
P3-B9		0.02763	0.00000	0.00000	0.00000
P3-C1	Clostridium perfringens	5.57412	0.00000	24.02252	0.00000
P3-C10	Clostridium perfringens	0.71723	0.11029	14.57273	0.00000
P3-C11	Clostridium perfringens	1.63981	0.07242	49.21909	0.00000
P3-C12		0.11244	0.16934	0.02252	0.00000
P3-C2	Clostridium perfringens	0.73451	0.00000	89.24200	0.00000
P3-C3	Clostridium perfringens	1.07343	0.04509	99.95836	0.00000
P3-C4	Clostridium perfringens	0.53319	0.03920	75.70073	0.00000

Sequence Summary Report

P3-C5	Clostridium perfringens	0.41412	0.06213	100.00000	0.00000
P3-C6	Clostridium perfringens	0.77330	0.06612	95.72283	0.00000
P3-C7	Clostridium perfringens	0.24067	0.05611	97.00607	0.00000
P3-C8		0.13672	0.00000	0.03182	0.00000
P3-C9	Clostridium perfringens	0.05478	0.00000	73.88949	0.00000
P3-D1		0.96008	0.03758	0.78782	0.00000
P3-D10	Clostridium perfringens	0.32439	0.00000	72.36535	0.00000
P3-D11	Clostridium perfringens	0.48075	0.07814	98.89026	0.00000
P3-D12	Clostridium perfringens	2.17388	0.14828	38.81224	0.00000
P3-D2		0.07424	0.07785	0.16122	0.00000
P3-D3	Clostridium perfringens	0.76857	0.10536	100.00000	0.00000
P3-D4	Clostridium perfringens	1.15756	0.07215	99.25482	0.00000
P3-D5	Clostridium perfringens	1.62943	0.08049	45.94084	0.00000
P3-D6	Clostridium perfringens	1.04895	0.05123	87.27977	0.00000
P3-D7	Clostridium perfringens	0.07881	0.03989	29.77756	0.00000
P3-D8	Clostridium perfringens	0.95645	0.05630	49.13060	0.00000
P3-D9	Clostridium perfringens	0.69771	0.09575	45.30661	0.00000
P3-E1	Clostridium perfringens	6.35653	0.06872	95.91740	0.00000
P3-E10	Clostridium perfringens	0.11336	0.15894	46.89499	0.00000
P3-E11	Clostridium perfringens	0.85345	0.07484	94.27890	0.00000
P3-E12	Clostridium perfringens	0.12876	0.11144	77.43442	0.00000
P3-E2	Clostridium perfringens	5.96444	0.10204	1.50844	0.00000
P3-E3	Clostridium perfringens	0.23619	0.04408	90.97546	0.00000
P3-E4	Clostridium perfringens	0.66690	0.08194	1.20138	0.00000
P3-E5	Clostridium perfringens	0.68799	0.05956	20.97578	0.00000
P3-E6	Clostridium perfringens	0.79123	0.00000	47.18241	0.00000
P3-E7	Clostridium perfringens	0.61406	0.04279	16.54851	0.00000
P3-E8	Clostridium perfringens	0.20598	0.04937	99.63419	0.00000
P3-E9	Clostridium perfringens	1.50024	0.04180	15.39342	0.00000
P3-F1	Clostridium perfringens	0.79554	0.04375	41.33744	0.00000
P3-F10		0.39814	0.00000	0.37659	0.00000
P3-F11	Clostridium perfringens	1.94334	0.03782	74.48873	0.00000
P3-F12	Clostridium perfringens	0.12627	0.12733	51.94301	0.00000
P3-F2		0.94855	0.13978	0.03661	0.00000
P3-F3	Clostridium perfringens	0.29007	0.00000	82.98616	0.00000
P3-F4	Clostridium perfringens	0.10861	0.15433	4.76170	0.00000
P3-F5	Clostridium perfringens	0.23673	0.03057	98.11292	0.00000

Sequence Summary Report

P3-F6	Clostridium perfringens	1.08508	0.71104	4.88340	0.00000
P3-F7	Clostridium perfringens	0.01983	25.57211	2.60407	97.39593
P3-F8	Ruminococcus gnavus	0.18143	27.10880	52.49258	46.14957
P3-F9	Clostridium perfringens	0.38468	0.00000	98.81418	0.00000
P3-G1	Clostridium perfringens	0.23529	0.03248	22.90683	0.00000
P3-G10	Clostridium perfringens	1.14055	0.05183	97.08495	0.00000
P3-G11	Clostridium perfringens	0.33132	27.73381	0.78034	98.35997
P3-G12		0.04911	0.06980	0.18124	0.29218
P3-G2	Ruminococcus gnavus	0.24153	22.18868	48.42299	43.77997
P3-G3	Clostridium perfringens	0.58240	0.00000	32.75538	0.00000
P3-G4	Clostridium perfringens	0.61205	0.06516	36.90437	0.00000
P3-G5	Clostridium perfringens	0.53059	0.05577	43.83541	0.00000
P3-G6	Clostridium perfringens	0.04822	0.11764	98.49617	0.00000
P3-G7	Clostridium perfringens	0.03987	0.08650	100.00000	0.00000
P3-G8	Clostridium perfringens	0.74578	0.05977	67.48157	0.00000
P3-G9	Clostridium perfringens	1.08321	0.07836	99.88428	0.00000
P3-H1	Clostridium perfringens	0.30252	0.08074	20.71473	0.00000
P3-H10		0.06888	0.06570	0.02478	0.00000
P3-H11		0.10529	0.00000	0.00000	0.00000
P3-H12		0.04466	0.06503	0.00000	0.00000
P3-H2	Clostridium perfringens	0.83888	0.04650	99.51622	0.00000
P3-H3	Clostridium perfringens	0.09169	0.00000	10.12035	0.00000
P3-H4	Clostridium perfringens	0.65165	0.03291	100.00000	0.00000
P3-H5	Clostridium perfringens	0.81587	0.46591	98.96462	0.00000
P3-H6	Clostridium perfringens	1.81324	0.04175	25.68884	0.00000
P3-H7	Clostridium perfringens	0.08223	0.00000	13.78581	0.00000
P3-H8	Clostridium perfringens	0.87914	0.20223	99.77441	0.00000
P3-H9		0.05896	0.00000	0.00000	0.00000

- PLATE4

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate4	**16S rDNA sequencing**	**3-OxoLCA production (%)**	**isoLCA production (%)**	**LCA production (%)**	**isoLCA production (%)**
P4-A1	**Roseburia faecis**	0.04131	0.06218	10.64598	2.68225
P4-A10		0.00000	0.00000	0.22471	0.11792
P4-A11		0.00000	0.06980	0.52897	0.00000
P4-A12		0.13686	0.00000	0.00000	0.00000
P4-A2		0.02931	0.00000	0.00000	0.00000
P4-A3		0.00000	0.08458	0.00000	0.00000
P4-A4		0.00000	0.09108	0.00000	0.07221
P4-A5		0.00000	0.05421	0.00000	0.00000
P4-A6		0.03343	0.00000	0.00000	0.00000
P4-A7	**Bacillus coagulans**	0.00000	0.00000	0.17659	53.55268
P4-A8	**Bacillus coagulans**	0.09968	0.00000	0.21065	64.15554
P4-A9	**Roseburia faecis**	0.02208	0.00000	88.76916	5.42824
P4-B1	**Clostridium aldenense**	0.24958	0.00000	3.37946	16.66502
P4-B10	**Phocea massiliensis**	1.32086	0.07467	86.42320	3.39077
P4-B11		0.00000	0.00000	0.00000	0.00000
P4-B12		0.09366	0.00000	0.00000	0.00000
P4-B2	**Clostridium aldenense**	2.17636	0.76229	34.88247	61.22177
P4-B3		0.02809	0.05109	0.00000	0.08333
P4-B4		0.00000	0.10525	0.00000	0.00000
P4-B5		0.00000	0.00000	0.00000	0.00000
P4-B6		0.00000	0.00000	0.00000	0.00000
P4-B7		0.00000	0.09794	0.00000	0.00000
P4-B8		0.10434	0.08155	0.32707	0.00000
P4-B9		0.11091	0.00000	0.20501	0.00000
P4-C1		0.63381	0.00000	0.00000	0.00000
P4-C10	**Clostridium citroniae**	0.07761	0.00000	88.42194	4.94213
P4-C11		0.08862	0.00000	0.54059	0.53067
P4-C12	**Bacteroides fragilis**	0.00000	0.00000	86.85391	0.21107
P4-C2		0.05000	0.00000	0.18937	5.52353
P4-C3		0.00000	0.07861	0.00000	0.00000
P4-C4		0.04253	0.00000	0.00000	0.00000

Sequence Summary Report

P4-C5		0.00000	0.08674	0.00000	0.00000
P4-C6		0.00000	0.07933	0.00000	0.00000
P4-C7		0.13754	0.00000	0.00000	0.00000
P4-C8		0.03823	0.00000	0.00000	0.00000
P4-C9		0.34134	0.08930	0.61111	0.56821
P4-D1	**Fusicatenibacter saccharivorans**	0.03713	0.05281	96.15253	3.51286
P4-D10		0.05479	0.00000	0.00000	0.00000
P4-D11		0.00000	0.00000	0.00000	0.00000
P4-D12		0.05575	0.03772	0.00000	0.00000
P4-D2		0.00000	0.09721	0.00000	0.00000
P4-D3		0.00000	0.10769	0.00000	0.00000
P4-D4		0.00000	0.17380	0.00000	0.00000
P4-D5		0.00000	0.00000	0.00000	0.00000
P4-D6	**Clostridium aldenense**	0.66174	0.10490	18.28490	4.51408
P4-D7		0.21615	0.00000	0.00000	0.00000
P4-D8		0.00000	0.06668	0.00000	0.00000
P4-D9		0.00000	0.18756	0.00000	0.00000
P4-E1		0.03683	0.00000	0.00000	0.00000
P4-E10		0.36658	0.00000	0.00000	0.00000
P4-E11		0.10058	0.08605	0.00000	0.00000
P4-E12		0.08287	0.25604	0.00000	0.00000
P4-E2	**Romboutsia lituseburensis**	0.00000	0.06973	11.68166	13.29531
P4-E3		0.11122	0.00000	0.00000	0.00000
P4-E4	**Romboutsia timonensis**	0.09589	0.11567	10.78270	1.10043
P4-E5	**Bacteroides fragilis**	0.00000	0.07495	7.24833	1.54549
P4-E6		0.08421	0.08216	0.00000	0.00000
P4-E7		0.00000	0.00000	0.00000	0.00000
P4-E8		0.00000	0.07612	0.00000	0.00000
P4-E9		0.12054	0.00000	0.00000	0.00000
P4-F1		0.44095	0.57193	0.00000	0.00000
P4-F10	**Clostridium perfringens**	21.62110	0.03675	93.58619	0.49505
P4-F11	**Clostridium perfringens**	15.86673	0.07946	81.61440	0.32529
P4-F12	**Clostridium perfringens**	6.26080	0.24302	82.76126	0.47362
P4-F2		0.00000	0.00000	0.00000	0.00000
P4-F3		0.00000	0.00000	0.03490	0.00000
P4-F4		0.00000	0.00000	0.00000	0.00000
P4-F5		0.00000	0.06903	0.00000	0.00000

Sequence Summary Report

P4-F6	**Clostridium perfringens**	2.43789	0.07638	96.35296	0.00000
P4-F7	**Clostridium perfringens**	1.31019	0.00000	92.41206	0.24208
P4-F8	**Clostridium aldenense**	2.70961	0.44668	32.66861	6.71354
P4-F9	**Clostridium perfringens**	0.10195	0.04457	9.85060	0.18221
P4-G1	**Clostridium perfringens**	3.06696	0.00000	83.72991	0.24167
P4-G10	**Clostridium perfringens**	2.76120	0.00000	90.75036	0.15843
P4-G11	**Clostridium perfringens**	16.70926	0.05442	88.09501	0.45870
P4-G12	**Clostridium perfringens**	38.33151	0.19432	88.81575	0.46315
P4-G2	**Ruminococcus gnavus**	0.68704	19.13871	73.00227	23.67676
P4-G3	**Clostridium perfringens**	34.02939	0.04036	86.32963	1.08307
P4-G4	**Clostridium perfringens**	29.73023	0.00000	90.96978	0.56736
P4-G5	**Clostridium perfringens**	33.17728	0.00000	91.14764	0.40673
P4-G6	**Clostridium perfringens**	26.80538	0.00000	89.99235	0.15519
P4-G7	**Clostridium perfringens**	20.99210	0.00000	90.88960	0.37955
P4-G8	**Clostridium perfringens**	12.21771	0.00000	97.80056	0.00000
P4-G9	**Clostridium perfringens**	21.50584	0.02950	96.73967	0.34898
P4-H1	**Clostridium perfringens**	34.20743	0.00000	84.64784	0.41899
P4-H10	**Clostridium perfringens**	2.29594	0.00000	93.13971	0.60197
P4-H11	**Clostridium perfringens**	3.34450	0.10198	87.11719	0.15687
P4-H12	**Clostridium perfringens**	22.41180	0.00000	93.25305	0.34212
P4-H2	**Clostridium perfringens**	1.68172	0.16722	89.76903	0.15412
P4-H3	**Clostridium perfringens**	2.44717	0.00000	87.56843	0.16944
P4-H4	**Clostridium perfringens**	1.72430	0.10102	88.99064	0.12301
P4-H5	**Clostridium perfringens**	2.00302	0.04339	96.00979	0.26234
P4-H6	**Clostridium perfringens**	24.30641	0.02946	88.94044	0.47597
P4-H7	**Clostridium perfringens**	28.92956	0.04700	92.33367	6.61562
P4-H8	**Coprobacillus cateniformis**	0.25859	0.00000	99.13505	0.00000
P4-H9	**Clostridium perfringens**	1.64309	0.24424	88.99835	0.17231

- PLATE5

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate5	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P5-A1	Collinsella aerofaciens	6.35832	0.17785	100.00000	0.00000
P5-A10	Collinsella aerofaciens	0.00000	0.00000	7.83984	0.48520
P5-A11		0.00000	0.13360	0.05129	0.00000
P5-A12	Bacteroides cellulosilyticus	0.00000	0.24641	12.08809	40.28507
P5-A2	Bifidobacterium longum	0.16383	1.34041	0.02586	1.99457
P5-A3	Collinsella aerofaciens	4.48771	0.00000	99.43387	0.00000
P5-A4		0.00000	0.27769	0.00000	47.46135
P5-A5	Peptoniphilus harei	0.00000	0.00000	1.91468	82.43851
P5-A6		0.00000	0.00000	0.00000	24.12213
P5-A7		0.10067	0.33789	0.31795	2.08422
P5-A8		0.50229	0.26525	0.60464	1.85514
P5-A9	Collinsella aerofaciens	3.29954	0.46866	93.94722	0.00000
P5-B1		0.00000	0.00000	0.00000	0.00000
P5-B10	Collinsella aerofaciens	0.51554	0.61793	99.75056	0.13289
P5-B11		0.00000	0.51917	0.00000	0.00000
P5-B12	Bacteroides cellulosilyticus	0.00000	0.00000	11.27135	0.71933
P5-B2		0.00000	0.73827	0.00000	0.00000
P5-B3	Collinsella aerofaciens	0.00000	0.93371	7.44576	0.55707
P5-B4		0.12778	0.86557	0.00000	0.00000
P5-B5		0.00000	0.00000	0.00000	0.00000
P5-B6	Collinsella aerofaciens	0.00000	0.37197	1.76918	93.87159
P5-B7	Collinsella aerofaciens	0.21324	0.00000	99.94257	0.00000
P5-B8		0.00000	0.00000	0.00000	0.06868
P5-B9	Bifidobacterium longum	1.47636	2.29794	2.36788	7.56313
P5-C1	Collinsella aerofaciens	4.16783	0.00000	47.03655	0.00000
P5-C10		0.00000	0.41384	0.00000	0.10701
P5-C11	Bifidobacterium longum	0.75415	2.16399	0.09530	3.46336
P5-C12		0.00000	0.00000	0.00000	0.00000
P5-C2	Collinsella aerofaciens	0.29273	6.13747	89.01105	8.91820
P5-C3		0.00000	0.00000	0.03648	10.35777
P5-C4	Bifidobacterium longum	1.45408	2.12153	0.04816	4.52518

Sequence Summary Report

P5-C5	**Collinsella aerofaciens**	0.00000	0.00000	10.42374	0.62101
P5-C6		0.00000	0.15480	0.00000	0.00000
P5-C7	**Collinsella aerofaciens**	0.00000	0.00000	9.41029	0.72405
P5-C8		0.00000	0.00000	0.01172	0.00000
P5-C9		0.00000	0.67108	0.00000	0.00000
P5-D1	**Collinsella aerofaciens**	0.00000	0.28006	14.56738	1.56613
P5-D10		1.59360	12.22718	0.04800	0.00000
P5-D11	**Collinsella aerofaciens**	0.70233	0.00000	99.32288	0.00000
P5-D12		0.52481	0.18082	0.24355	4.30147
P5-D2		0.00000	0.00000	0.00000	2.28786
P5-D3		0.09161	0.28118	0.00000	0.28634
P5-D4		0.07542	0.28662	0.00000	0.00000
P5-D5	**Collinsella aerofaciens**	0.82951	0.00000	99.39542	0.00000
P5-D6		0.00000	0.00000	0.00000	0.00000
P5-D7		0.00000	0.30827	0.05379	0.72024
P5-D8		0.00000	0.30035	0.06145	7.37611
P5-D9	**Collinsella aerofaciens**	0.00000	0.00000	5.78695	1.77300
P5-E1	**Bacteroides dorei**	0.00000	0.00000	1.79280	0.98924
P5-E10		0.00000	0.00000	0.00000	0.10101
P5-E11	**Bacteroides cellulosilyticus**	0.00000	0.00000	96.62218	0.83395
P5-E12	**Bifidobacterium pseudocatenulatum**	0.00000	0.32475	12.02219	64.21384
P5-E2		1.61618	0.65487	0.13583	10.44787
P5-E3	**Bifidobacterium longum**	1.45199	2.02448	2.74125	5.82997
P5-E4		0.00000	0.52835	0.22599	18.22831
P5-E5	**Bifidobacterium longum**	0.08819	2.09533	3.56424	0.47473
P5-E6	**Bifidobacterium longum**	1.27046	2.26067	25.94907	72.32475
P5-E7		0.09179	0.44059	0.05398	0.48957
P5-E8	**Collinsella aerofaciens**	0.64140	0.60553	99.96220	0.00000
P5-E9	**Collinsella aerofaciens**	0.00000	0.55511	11.92025	0.81696
P5-F1		0.10068	0.00000	0.00000	1.54274
P5-F10		0.00000	0.00000	0.00000	3.91072
P5-F11		0.00000	0.00000	0.02656	6.92200
P5-F12	**Bifidobacterium longum**	0.09506	2.23312	1.80464	95.41979
P5-F2	**Collinsella aerofaciens**	1.22242	0.00000	100.00000	0.00000
P5-F3	**Bifidobacterium longum**	0.20974	1.02181	0.03011	2.32614
P5-F4		0.00000	0.25372	0.00000	0.00000
P5-F5	**Bifidobacterium faecale**	0.00000	0.22998	1.14343	0.00000

Sequence Summary Report

P5-F6	Collinsella aerofaciens	0.00000	0.00000	6.84434	70.72986
P5-F7	Collinsella aerofaciens	0.28076	0.56239	100.00000	0.00000
P5-F8		0.00000	0.00000	0.09846	0.40862
P5-F9		0.00000	0.34488	0.00000	0.00000
P5-G1	Bacteroides cellulosilyticus	1.68478	0.00000	97.84053	0.00000
P5-G10	Collinsella aerofaciens	0.35874	0.00000	2.64588	0.00000
P5-G11	Bacteroides cellulosilyticus	0.00000	0.00000	0.36476	95.67585
P5-G12	Bifidobacterium faecale	0.00000	0.00000	19.20505	0.00000
P5-G2	Collinsella aerofaciens	0.23720	0.00000	99.87347	0.00000
P5-G3	Bifidobacterium longum	1.80020	2.33632	0.04824	5.57488
P5-G4	Collinsella aerofaciens	0.31259	0.00000	99.92285	0.05581
P5-G5	Collinsella aerofaciens	0.23247	0.81635	24.24741	0.00000
P5-G6	Bifidobacterium longum	1.51745	0.77337	26.56201	71.91720
P5-G7	Bifidobacterium longum	0.14271	2.01638	3.64790	5.26859
P5-G8		0.00000	0.20980	0.10540	86.94181
P5-G9		0.00000	0.00000	0.00000	0.72537
P5-H1		0.00000	0.00000	0.00000	19.76039
P5-H10		0.00000	0.21221	0.00000	0.00000
P5-H11	Bacteroides fragilis	2.75009	0.00000	3.83345	0.00000
P5-H12	Bacteroides fragilis	31.03629	0.00000	98.30083	0.00000
P5-H2		0.00000	0.12643	0.00000	99.39552
P5-H3		0.00000	0.64587	0.05376	0.00000
P5-H4		0.00000	0.27373	0.00000	0.00000
P5-H5		0.00000	0.29779	0.00000	0.10413
P5-H6	Collinsella intestinalis	4.58706	0.67423	96.97683	0.00000
P5-H7		0.00000	0.27028	0.00000	0.00000
P5-H8	Bifidobacterium pseudocatenulatum	0.00000	0.18864	0.00000	70.84122
P5-H9	Bacteroides fragilis	0.00000	0.00000	0.36897	14.99881

- **PLATE6**

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate6	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P6-A1		0.04739	0.00000	0.00000	0.00000
P6-A10	Collinsella intestinalis	5.03699	0.05249	80.87789	0.20138
P6-A11	Collinsella intestinalis	2.18681	0.05554	80.95377	0.23985
P6-A12	Collinsella intestinalis	0.78213	0.00000	88.92832	0.16588
P6-A2	Collinsella intestinalis	0.79731	0.03464	82.57390	0.15288
P6-A3	Peptoniphilus harei	0.00000	0.03797	4.83845	83.78978
P6-A4		0.00000	0.03637	0.06501	0.00000
P6-A5	Collinsella aerofaciens	0.09483	0.05829	80.81056	0.00000
P6-A6		0.00000	0.09777	0.03097	0.00000
P6-A7	Collinsella intestinalis	0.05779	0.09028	85.02009	0.14596
P6-A8	Collinsella intestinalis	1.13690	0.00000	85.78117	0.00000
P6-A9	Peptoniphilus harei	0.00000	0.00000	5.44749	77.61245
P6-B1	Collinsella intestinalis	0.73471	0.61133	85.10960	0.08380
P6-B10	Collinsella intestinalis	3.17529	0.03265	80.95873	0.00000
P6-B11	Collinsella intestinalis	0.83753	0.07194	87.66914	0.22560
P6-B12	Collinsella intestinalis	0.81978	0.00000	86.39735	0.31679
P6-B2	Collinsella intestinalis	0.74456	0.00000	86.24369	0.28054
P6-B3	Collinsella intestinalis	0.75311	0.11385	89.46062	0.26828
P6-B4	Collinsella intestinalis	0.04970	0.04470	81.48347	0.34738
P6-B5	Collinsella intestinalis	1.21965	0.00000	86.81133	0.00000
P6-B6	Peptoniphilus harei	0.00000	0.00000	18.34299	20.28317
P6-B7	Collinsella aerofaciens	0.02406	0.08259	78.76877	0.26058
P6-B8	Collinsella intestinalis	1.09642	0.03280	90.20711	0.11975
P6-B9	Collinsella intestinalis	1.50241	0.07474	85.28664	0.00000
P6-C1	Collinsella intestinalis	0.06323	0.00000	90.75315	0.15363
P6-C10	Collinsella intestinalis	1.26260	0.00000	84.35965	0.36637
P6-C11	Collinsella intestinalis	0.08661	0.08183	84.84703	0.53000
P6-C12		0.00000	0.00000	0.59619	0.00000
P6-C2	Collinsella intestinalis	0.96269	0.00000	88.12759	0.34382
P6-C3	Collinsella intestinalis	1.76012	0.05587	83.43802	0.13792
P6-C4	Collinsella intestinalis	0.07054	0.10732	90.44832	0.08360

Sequence Summary Report

P6-C5	Collinsella intestinalis	1.09067	0.00000	90.76124	0.00000
P6-C6	Eggerthella lenta	9.72812	19.75481	22.88320	6.79556
P6-C7	Peptoniphilus harei	0.06349	0.08096	87.33350	0.00000
P6-C8	Collinsella intestinalis	0.06119	0.04519	90.22181	0.08504
P6-C9	Collinsella intestinalis	0.37149	0.00000	87.54129	0.00000
P6-D1	Bacteroides cellulosilyticus	0.00000	0.10404	0.26346	29.34336
P6-D10	Bacteroides vulgatus	0.00000	0.09198	5.27356	25.00190
P6-D11		0.00000	0.08321	0.00000	0.00000
P6-D12	Bifidobacterium longum	0.00000	0.00000	17.08818	26.07555
P6-D2	Collinsella aerofaciens	0.00000	0.07956	43.76892	9.46219
P6-D3	Collinsella aerofaciens	0.42278	0.06742	88.72734	0.29577
P6-D4	Bifidobacterium longum	0.00000	0.00000	16.75673	23.60516
P6-D5		0.00000	0.00000	0.10158	0.41138
P6-D6		0.00000	0.06727	0.11505	0.00000
P6-D7		0.00000	0.00000	0.09090	0.00000
P6-D8		0.00000	0.00000	0.10317	0.36630
P6-D9	Collinsella aerofaciens	0.00000	0.04473	43.08762	7.73917
P6-E1	Collinsella aerofaciens	0.48776	0.04171	85.87531	0.26055
P6-E10		0.00000	0.06279	0.08149	0.00000
P6-E11	Bifidobacterium longum	0.00000	0.00000	17.93394	26.84629
P6-E12		0.00000	0.05864	0.11141	0.15901
P6-E2		0.00000	0.09794	0.12328	0.00000
P6-E3	Collinsella aerofaciens	0.02175	0.00000	87.36951	0.29076
P6-E4	Collinsella aerofaciens	0.00000	0.00000	85.35505	0.46543
P6-E5		0.00000	0.05088	0.00000	0.13020
P6-E6		0.04599	0.00000	0.07757	0.00000
P6-E7	Collinsella aerofaciens	0.07318	0.00000	81.12988	0.14626
P6-E8		0.04474	0.00000	0.02863	18.39104
P6-E9		0.02917	0.00000	0.00000	0.07482
P6-F1	Collinsella aerofaciens	0.12430	0.04989	88.38759	0.32333
P6-F10	Bacteroides uniformis/ Bacteroides rodentium	0.00000	0.00000	0.00000	35.35425
P6-F11		0.00000	0.00000	0.14505	0.19331
P6-F12	Bacteroides cellulosilyticus	0.00000	0.00000	0.02763	32.41464
P6-F2	Bifidobacterium longum	0.00000	0.00000	5.72530	10.11808
P6-F3	Bifidobacterium longum	0.03621	0.00000	16.23888	25.21364
P6-F4	Collinsella aerofaciens	0.07799	0.05097	88.65441	0.34582
P6-F5		0.00000	0.00000	0.10286	0.20780

Sequence Summary Report

P6-F6	Collinsella aerofaciens	0.23472	0.12534	88.77833	0.10917
P6-F7		0.06347	0.00000	0.12063	0.15586
P6-F8	Collinsella aerofaciens	0.00000	0.04827	45.05085	9.34177
P6-F9		0.00000	0.06564	0.04082	0.20986
P6-G1	Bacteroides fragilis	0.00000	0.00000	1.35950	45.10501
P6-G10		0.00000	0.00000	0.04410	1.43551
P6-G11	Collinsella aerofaciens	0.09276	0.00000	82.71868	0.27251
P6-G12		0.00000	0.00000	0.00000	0.14902
P6-G2	Collinsella aerofaciens	0.10549	0.04649	83.05247	0.24624
P6-G3	Bacteroides cellulosilyticus	0.00000	0.10601	0.04566	46.84486
P6-G4	Collinsella aerofaciens	0.00000	0.00000	45.99707	8.15475
P6-G5	Collinsella aerofaciens	0.04633	0.00000	86.13539	0.36727
P6-G6		0.00000	0.00000	0.00000	0.00000
P6-G7		0.00000	0.08702	0.19198	1.95192
P6-G8	Bacteroides cellulosilyticus	0.00000	0.28700	0.10881	31.92564
P6-G9		0.00000	0.04707	0.16848	0.14682
P6-H1	Bacteroides fragilis	0.00000	0.00000	2.23577	47.41220
P6-H10	Bifidobacterium longum	0.00000	0.07649	5.39632	9.60726
P6-H11		0.00000	0.00000	0.07380	0.00000
P6-H12		0.03280	0.06039	0.00000	0.00000
P6-H2	Collinsella aerofaciens	0.00000	0.00000	53.59665	9.13661
P6-H3	Bifidobacterium longum	0.02946	0.00000	14.06397	22.14646
P6-H4		0.00000	0.06995	0.00000	0.00000
P6-H5	Bacteroides dorei	0.00000	0.10640	8.96245	19.19089
P6-H6		0.27899	0.00000	0.15487	0.57411
P6-H7	Collinsella aerofaciens	0.05950	0.05554	11.40488	6.62472
P6-H8		0.03547	0.00000	0.00000	0.00000
P6-H9		0.00000	0.16372	0.54537	32.22356

- PLATE7

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate7	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P7-A1		0.00000	0.00000	0.00000	0.08149
P7-A10	Collinsella intestinalis	2.12578	0.00000	83.82000	0.28239
P7-A11	Collinsella intestinalis	2.08956	0.03026	86.53722	0.78321
P7-A12	Collinsella intestinalis	2.47589	0.00000	87.65660	0.97189
P7-A2	Raoultibacter massiliensis	10.90595	0.02497	44.33729	0.16447
P7-A3	Collinsella intestinalis	2.15431	0.02110	83.68233	0.00000
P7-A4	Collinsella intestinalis	1.33325	0.03000	86.22256	0.09864
P7-A5		0.01376	0.00000	0.09730	0.00000
P7-A6	Collinsella intestinalis	0.40948	0.05383	88.34519	0.09547
P7-A7		0.00000	0.00000	0.05505	0.00000
P7-A8	Collinsella intestinalis	1.51431	0.00000	89.24219	1.33112
P7-A9	Collinsella intestinalis	2.77175	0.00000	89.11561	0.29084
P7-B1	Collinsella intestinalis	1.27907	0.00000	86.15241	0.13486
P7-B10	Peptoniphilus harei	0.00000	0.00000	6.05415	78.48273
P7-B11	Collinsella intestinalis	1.93719	0.00000	86.48642	0.63739
P7-B12	Collinsella intestinalis	1.33037	0.00000	89.83860	0.47198
P7-B2	Collinsella intestinalis	1.88057	0.00000	89.96373	0.00000
P7-B3	Collinsella aerofaciens	0.73715	0.09642	85.48110	0.00000
P7-B4	Collinsella intestinalis	1.34818	0.00000	90.60103	0.31750
P7-B5	Collinsella intestinalis	1.13056	0.00000	90.81693	0.38595
P7-B6	Peptoniphilus harei	0.00000	0.00000	4.57459	82.98978
P7-B7	Collinsella intestinalis	0.87547	0.00000	91.63545	0.00000
P7-B8	Peptoniphilus harei	0.00000	0.01662	5.33779	78.89307
P7-B9	Collinsella intestinalis	3.04259	0.04234	93.14118	0.20256
P7-C1	Collinsella intestinalis	1.87849	0.00000	87.22774	0.24323
P7-C10	Collinsella intestinalis	2.02710	0.04405	90.02566	0.21949
P7-C11	Peptoniphilus harei	0.01055	0.01592	4.60605	85.01845
P7-C12	Peptoniphilus harei	0.00000	0.00000	5.45745	82.41179
P7-C2	Collinsella intestinalis	0.81303	0.00000	92.60209	0.29581
P7-C3	Peptoniphilus harei	0.00000	0.00000	6.02837	68.62382
P7-C4	Collinsella intestinalis	0.69611	0.00000	93.53722	0.24009

Sequence Summary Report

P7-C5	Collinsella intestinalis	0.91133	0.00000	94.41519	0.30115
P7-C6	Collinsella intestinalis	1.22687	0.00000	93.63386	0.18295
P7-C7	Collinsella intestinalis	0.06364	0.00000	93.61567	0.20943
P7-C8	Collinsella intestinalis	0.03371	0.00000	92.56804	0.41874
P7-C9	Collinsella intestinalis	0.26536	0.00000	93.64264	0.22941
P7-D1	Collinsella intestinalis	2.41715	0.01726	90.66354	0.28759
P7-D10	Collinsella intestinalis	0.04593	0.03971	92.22222	0.27757
P7-D11	Collinsella intestinalis	3.30840	0.00000	91.51434	0.27907
P7-D12	Collinsella intestinalis	1.38002	0.00000	92.70704	0.00000
P7-D2	Collinsella intestinalis	3.40013	0.00000	95.32890	0.00000
P7-D3	Collinsella intestinalis	2.66549	0.00000	94.46089	0.35258
P7-D4	Collinsella intestinalis	1.19199	0.04695	92.95004	0.09506
P7-D5	Collinsella intestinalis	1.87314	0.00000	95.63740	0.13336
P7-D6	Collinsella intestinalis	0.05907	0.00000	94.85396	0.29450
P7-D7	Collinsella intestinalis	0.21167	0.00000	93.29147	0.35016
P7-D8	Collinsella intestinalis	0.61819	0.00000	93.07241	0.25222
P7-D9	Collinsella intestinalis	1.49679	0.00000	95.15976	0.17585
P7-E1	Collinsella intestinalis	4.98890	0.00000	88.38053	0.22665
P7-E10	Collinsella intestinalis	0.27568	0.09186	92.58653	0.20042
P7-E11	Collinsella intestinalis	1.63905	0.03831	92.41037	0.00000
P7-E12	Collinsella intestinalis	1.21051	0.00000	89.24012	0.32901
P7-E2	Collinsella intestinalis	3.23527	0.00000	94.40808	0.33750
P7-E3	Gordonibacter pamelaeae	22.82634	3.64573	46.80347	16.49276
P7-E4	Collinsella intestinalis	0.05923	0.00000	94.41703	0.36419
P7-E5	Collinsella intestinalis	1.59325	0.04210	94.12225	0.27851
P7-E6	Collinsella intestinalis	0.15709	0.00000	95.40575	0.17234
P7-E7	Collinsella intestinalis	0.36160	0.00000	93.02594	0.00000
P7-E8	Collinsella intestinalis	2.34159	0.00000	93.28704	0.37041
P7-E9	Collinsella intestinalis	4.52619	0.00000	95.69402	0.00000
P7-F1	Collinsella intestinalis	4.13674	0.00000	89.59086	0.18593
P7-F10	Eggerthella lenta	6.84812	7.43788	17.86148	4.72162
P7-F11	Collinsella intestinalis	2.83460	0.05118	90.98127	0.29330
P7-F12	Collinsella intestinalis	0.49667	0.00000	90.12974	0.00000
P7-F2	Collinsella aerofaciens	0.00000	0.04336	55.87166	9.11060
P7-F3	Collinsella intestinalis	2.12561	0.00000	95.80454	0.26831
P7-F4	Collinsella intestinalis	0.93680	0.00000	94.96916	0.14224
P7-F5	Collinsella intestinalis	1.06129	0.00000	93.71275	0.29961

Sequence Summary Report

P7-F6	**Collinsella intestinalis**	0.48780	0.03590	97.99953	0.00000
P7-F7	**Collinsella intestinalis**	0.14085	0.05765	92.90184	0.21848
P7-F8	**Peptoniphilus harei**	0.00000	0.03670	5.40581	77.82719
P7-F9	**Collinsella intestinalis**	0.07258	0.00000	92.60414	0.34866
P7-G1	**Collinsella intestinalis**	8.86156	0.03543	91.46105	0.28099
P7-G10	**Collinsella intestinalis**	0.19588	0.00000	88.43309	0.26984
P7-G11	**Collinsella intestinalis**	0.05257	0.00000	87.56368	0.15353
P7-G12	**Monoglobus pectinilyticus**	0.19071	0.00000	29.96833	0.26837
P7-G2	**Collinsella intestinalis**	3.93531	0.00000	93.39960	0.28829
P7-G3	**Collinsella intestinalis**	3.42268	0.00000	92.52948	0.27991
P7-G4		0.00000	0.00000	0.00000	0.00000
P7-G5		0.00000	0.00000	0.00000	0.00000
P7-G6	**Collinsella intestinalis**	0.99822	0.00000	91.11152	0.27057
P7-G7	**Eggerthella lenta**	20.90626	3.87219	11.41579	3.47197
P7-G8		0.28227	0.00000	87.10975	0.23175
P7-G9	**Eggerthella lenta**	36.55302	47.54130	25.20126	7.50220
P7-H1		0.00000	0.00000	0.04876	0.00000
P7-H10	**Monoglobus pectinilyticus**	0.04172	0.00000	27.36535	0.23802
P7-H11	**Collinsella intestinalis**	0.36013	0.00000	80.45786	0.16247
P7-H12	**Peptoniphilus harei**	0.00000	0.00000	0.02855	87.94745
P7-H2	**Collinsella intestinalis**	2.68505	0.00000	91.02001	0.22526
P7-H3	**Collinsella intestinalis**	2.83854	0.00000	86.13365	0.08121
P7-H4	**Peptoniphilus harei**	0.00000	0.00000	4.88038	82.13127
P7-H5		0.18895	0.00000	0.02948	0.00000
P7-H6	**Collinsella intestinalis**	1.12293	0.00000	82.14284	0.09609
P7-H7	**Collinsella intestinalis**	0.12046	0.03505	85.77946	0.00000
P7-H8	**Collinsella intestinalis**	0.79596	0.00000	87.11181	0.15417
P7-H9	**Collinsella intestinalis**	0.06189	0.00000	87.97733	0.31982

- PLATE8

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate8	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P8-A1		0.02605	0.00000	0.11567	0.21029
P8-A10	Bifidobacterium longum	0.24630	0.07986	17.49833	26.42472
P8-A11	Collinsella aerofaciens	0.11551	0.10361	8.99470	5.57623
P8-A12	Collinsella aerofaciens	0.04131	0.10457	79.74763	0.13274
P8-A2	Bifidobacterium longum	0.09291	0.04534	16.59738	25.46388
P8-A3	Collinsella aerofaciens	0.03493	0.00000	49.90561	8.22788
P8-A4	Collinsella aerofaciens	0.00000	0.00000	84.23534	0.00000
P8-A5	Collinsella aerofaciens	0.15796	0.03469	48.69747	10.11218
P8-A6	Collinsella aerofaciens	0.05045	0.05990	83.43207	0.00000
P8-A7	Collinsella aerofaciens	0.04655	0.05439	77.04708	0.20146
P8-A8	Collinsella aerofaciens	0.02358	0.09240	81.20127	0.22826
P8-A9		0.09964	0.00000	0.06667	0.10516
P8-B1	Peptoniphilus harei	0.15435	0.12996	5.38119	76.32120
P8-B10		0.04593	0.04818	0.68866	0.12481
P8-B11	Collinsella intestinalis	5.66346	0.15010	85.24643	0.28681
P8-B12	Peptoniphilus harei	0.02900	0.07365	4.17572	82.19406
P8-B2	Peptoniphilus harei	0.00000	0.15806	5.64757	77.09931
P8-B3		0.03679	0.05010	0.00000	0.00000
P8-B4		0.07458	0.04139	0.42340	23.49654
P8-B5	Monoglobus pectinilyticus	0.28013	0.07043	33.09927	0.34213
P8-B6	Collinsella intestinalis	13.70085	0.05964	87.37722	0.00000
P8-B7	Peptoniphilus harei	0.03342	0.04146	5.61610	74.96311
P8-B8	Collinsella aerofaciens	0.06655	0.05562	85.90964	0.30073
P8-B9	Monoglobus pectinilyticus	2.49782	0.00000	32.55076	0.24425
P8-C1	Monoglobus pectinilyticus	4.17787	0.06604	36.30624	0.08437
P8-C10	Collinsella intestinalis	12.69198	0.05114	86.84912	0.27043
P8-C11	Monoglobus pectinilyticus	1.59023	0.00000	31.83882	0.20927
P8-C12	Collinsella intestinalis	21.10642	0.06973	86.36487	0.25369
P8-C2	Collinsella intestinalis	1.08661	0.00000	93.97437	0.22891
P8-C3	Collinsella intestinalis	15.04968	0.13271	94.27427	0.20884
P8-C4	Monoglobus pectinilyticus	0.34233	0.17082	35.61409	0.32007

P8-C5	Monoglobus pectinilyticus	0.25077	0.13682	32.48034	0.00000
P8-C6		0.02147	0.17407	0.03886	0.00000
P8-C7	Collinsella intestinalis	8.74024	0.02187	90.66014	0.25646
P8-C8	Monoglobus pectinilyticus	2.39225	0.16230	90.01398	0.08637
P8-C9	Collinsella intestinalis	1.45061	0.00000	90.83013	0.24617
P8-D1	Collinsella intestinalis	23.14536	0.00000	93.26084	0.13663
P8-D10	Monoglobus pectinilyticus	1.27344	0.03870	34.63793	0.29143
P8-D11	Peptoniphilus harei	0.12227	0.12020	4.62060	78.05975
P8-D12	Collinsella intestinalis	3.78555	0.00000	93.76057	0.00000
P8-D2	Eggerthella lenta	48.81447	8.13633	47.23950	22.06168
P8-D3	Collinsella intestinalis	12.84827	0.00000	93.06784	0.07164
P8-D4	Peptoniphilus harei	0.07175	0.00000	5.20410	76.24708
P8-D5	Collinsella intestinalis	3.89545	0.00000	94.34285	0.00000
P8-D6	Collinsella intestinalis	0.78667	0.00000	92.75317	0.00000
P8-D7	Monoglobus pectinilyticus	0.31686	0.00000	32.00372	0.22009
P8-D8	Eggerthella lenta	43.03595	9.90261	44.69670	17.64921
P8-D9		0.14188	0.00000	0.00000	0.00000
P8-E1		0.16003	0.09205	0.08349	0.00000
P8-E10	Collinsella intestinalis	6.31235	0.20942	89.26881	0.00000
P8-E11	Monoglobus pectinilyticus	1.27524	0.07853	36.88274	0.07824
P8-E12	Monoglobus pectinilyticus	1.30826	0.31534	37.08392	0.40482
P8-E2	Peptoniphilus harei	0.09433	0.00000	5.56548	73.71652
P8-E3		0.02717	0.00000	0.03038	0.00000
P8-E4	Monoglobus pectinilyticus	0.39670	0.21272	33.28813	0.23889
P8-E5	Collinsella intestinalis	4.68123	0.03457	94.03777	0.21820
P8-E6	Monoglobus pectinilyticus	0.72109	0.10450	31.29797	0.17059
P8-E7	Collinsella intestinalis	0.08094	0.16421	91.25153	0.00000
P8-E8	Peptoniphilus harei	0.00000	0.04227	5.51501	73.74883
P8-E9		0.13039	0.04484	0.04554	0.00000
P8-F1		0.17217	0.07425	0.00000	0.00000
P8-F10	Peptoniphilus harei	0.09541	0.11228	5.43071	76.19893
P8-F11	Peptoniphilus harei	3.30883	0.45147	0.02676	94.68729
P8-F12	Collinsella intestinalis	6.89357	0.14064	0.01545	96.39206
P8-F2	Eggerthella lenta	20.16405	11.92693	79.67543	17.84863
P8-F3	Eggerthella lenta	50.26139	10.12897	42.85667	17.01935
P8-F4	Monoglobus pectinilyticus	1.66689	0.05879	28.27532	0.00000
P8-F5	Peptoniphilus harei	0.00000	0.08212	5.00071	75.71169

Sequence Summary Report

P8-F6	**Peptoniphilus harei**	0.00000	0.04021	5.57630	73.55224
P8-F7	**Collinsella intestinalis**	7.33921	0.03838	90.50494	0.00000
P8-F8	**Collinsella intestinalis**	7.96172	0.03035	91.93853	0.00000
P8-F9	**Collinsella intestinalis**	5.17015	0.05536	93.09270	0.00000
P8-G1	**Eggerthella lenta**	45.25475	9.29648	35.89902	13.19238
P8-G10	**Peptoniphilus harei**	0.02419	0.07393	4.70986	77.53346
P8-G11	**Collinsella aerofaciens**	0.08311	0.05493	85.09003	0.24411
P8-G12	**Peptoniphilus harei**	0.98549	0.06522	42.51834	0.38487
P8-G2	**Eggerthella lenta**	0.04235	0.09199	88.44842	0.00000
P8-G3	**Peptoniphilus harei**	0.05769	0.00000	16.81608	21.53425
P8-G4	**Collinsella intestinalis**	0.04522	0.10061	86.12116	0.30557
P8-G5	**Monoglobus pectinilyticus**	1.21695	0.00000	34.66803	0.21776
P8-G6		0.20583	0.27653	0.50734	26.58322
P8-G7	**Collinsella intestinalis**	1.14283	0.06875	88.49695	0.19565
P8-G8	**Collinsella intestinalis**	0.94443	0.03972	89.67492	0.00000
P8-G9		0.06353	0.08582	0.00000	0.00000
P8-H1	**Monoglobus pectinilyticus**	3.10662	0.09463	42.75429	0.39168
P8-H10	**Monoglobus pectinilyticus**	1.16742	0.14987	30.50877	0.23948
P8-H11	**Monoglobus pectinilyticus**	0.59432	0.00000	30.63150	0.17592
P8-H12	**Peptoniphilus harei**	0.06031	0.05304	4.59360	80.87113
P8-H2	**Monoglobus pectinilyticus**	2.08661	0.08425	44.31678	0.31906
P8-H3	**Monoglobus pectinilyticus**	1.49068	0.04943	36.89020	0.37450
P8-H4	**Monoglobus pectinilyticus**	1.41018	0.03699	7.72229	2.56529
P8-H5	**Eggerthella lenta**	37.00561	14.29137	3.33597	1.08090
P8-H6	**Monoglobus pectinilyticus**	1.41475	0.12192	31.71054	0.08246
P8-H7		0.07230	0.00000	0.00000	0.00000
P8-H8	**Monoglobus pectinilyticus**	0.78278	0.26257	30.97117	0.06489
P8-H9	**Monoglobus pectinilyticus**	0.81762	0.00000	34.11502	0.22899

- PLATE9

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate9	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P9-A1	Collinsella intestinalis	7.28082	0.00000	99.07172	0.00000
P9-A10	Collinsella intestinalis	4.40681	0.00000	98.39648	0.00000
P9-A11	Collinsella intestinalis	4.18293	0.00000	90.20278	0.00000
P9-A12	Collinsella intestinalis	5.77091	0.00000	98.97189	0.00000
P9-A2	Collinsella intestinalis	3.96405	0.00000	99.39062	0.51599
P9-A3		0.00000	0.05769	0.00000	0.00000
P9-A4		0.07546	0.00000	0.00000	0.00000
P9-A5	Collinsella intestinalis	2.56883	0.07237	99.74925	0.00000
P9-A6	Collinsella intestinalis	2.70121	0.06270	99.14807	0.00000
P9-A7	Collinsella intestinalis	0.80434	0.00000	99.30726	0.00000
P9-A8	Collinsella intestinalis	2.28450	0.00000	98.01761	0.29373
P9-A9	Collinsella intestinalis	3.19246	0.09187	99.20526	0.00000
P9-B1	Collinsella intestinalis	4.39110	0.09839	96.18479	0.20904
P9-B10	Collinsella aerofaciens	0.00000	0.00000	15.12151	2.67324
P9-B11	Bifidobacterium longum	0.05328	0.07403	0.00000	97.24012
P9-B12		0.00000	0.06169	0.00000	0.12563
P9-B2	Collinsella intestinalis	6.02249	0.13259	98.65584	0.17824
P9-B3	Peptoniphilus harei	0.00000	0.00000	2.62904	40.49974
P9-B4	Bifidobacterium longum	0.03795	0.00000	2.40203	5.02133
P9-B5		0.00000	0.05663	0.00000	3.47494
P9-B6	Collinsella aerofaciens	0.08775	0.00000	99.72768	0.00000
P9-B7	Collinsella aerofaciens	0.00000	0.00000	17.07097	2.63041
P9-B8		0.03520	0.00000	0.00000	0.00000
P9-B9		0.04006	0.00000	0.00000	0.00000
P9-C1		0.00000	0.00000	0.00000	0.00000
P9-C10	Bifidobacterium longum	0.07964	0.00000	1.88794	3.55003
P9-C11	Bifidobacterium longum	0.09238	0.00000	24.48863	43.94762
P9-C12	Collinsella aerofaciens	0.69941	0.00000	97.11219	0.90159
P9-C2	Parolsenella catena	0.00000	0.07356	0.81275	95.04366
P9-C3		0.00000	0.00000	0.00000	0.00000
P9-C4		0.00000	0.00000	0.00000	3.06098

Sequence Summary Report

P9-C5		0.04963	0.09247	0.03656	0.00000
P9-C6		0.04087	0.05772	0.91301	1.61369
P9-C7		0.00000	0.00000	0.00000	4.85521
P9-C8	**Parolsenella catena**	0.00000	0.00000	0.11359	96.75234
P9-C9	**Parabacteroides distasonis**	0.08782	0.72376	2.67119	41.39989
P9-D1		0.00000	0.09846	0.32721	0.12020
P9-D10		0.00000	0.00000	0.00000	0.00000
P9-D11		0.05300	0.00000	0.00000	0.00000
P9-D12	**Collinsella aerofaciens**	0.63862	0.12399	98.69657	0.13602
P9-D2	**Collinsella aerofaciens**	0.00000	0.00000	14.88628	2.49990
P9-D3		0.00000	0.08075	0.00000	0.00000
P9-D4	**Collinsella aerofaciens**	0.05718	0.00000	98.91456	0.00000
P9-D5	**Parolsenella catena**	0.03272	0.08326	0.43914	97.18028
P9-D6		0.00000	0.00000	0.03597	0.00000
P9-D7		0.00000	0.09548	0.08559	11.99631
P9-D8	**Collinsella aerofaciens**	0.13098	0.00000	99.11986	0.11436
P9-D9	**Parabacteroides chongii**	0.00000	0.00000	0.08285	16.12584
P9-E1		0.00000	0.13739	0.00000	0.00000
P9-E10		0.00000	0.05884	0.00000	0.07089
P9-E11	**Bifidobacterium longum**	0.00000	0.00000	1.14001	3.40083
P9-E12		0.03352	0.06095	0.00000	0.00000
P9-E2		0.00000	0.06122	0.00000	0.00000
P9-E3	**Collinsella aerofaciens**	0.59485	0.11064	95.54359	0.00000
P9-E4		0.00000	0.00000	0.02774	0.00000
P9-E5		0.00000	0.00000	0.00000	0.00000
P9-E6	**Collinsella aerofaciens**	0.00000	0.05504	23.01025	4.02213
P9-E7		0.00000	0.00000	0.02937	0.00000
P9-E8		0.00000	0.00000	0.03200	0.10620
P9-E9		0.00000	0.00000	0.00000	7.37578
P9-F1	**Bifidobacterium longum**	0.04859	0.00000	2.24862	4.15510
P9-F10	**Collinsella intestinalis**	10.64282	0.70182	94.95824	0.00000
P9-F11	**Peptoniphilus harei**	0.00000	0.00000	3.51141	40.56271
P9-F12	**Collinsella intestinalis**	4.96933	0.00000	94.11615	0.47160
P9-F2	**Collinsella intestinalis**	3.68657	0.06006	97.69122	0.00000
P9-F3	**Collinsella intestinalis**	4.91153	0.11714	96.51039	0.00000
P9-F4	**Collinsella intestinalis**	1.76157	0.00000	99.56819	0.15655
P9-F5	**Collinsella intestinalis**	2.78870	0.04439	96.61440	0.30722

Sequence Summary Report

P9-F6	**Collinsella intestinalis**	2.67907	0.00000	95.50631	0.27353
P9-F7	**Peptoniphilus harei**	0.00000	0.00000	4.24911	48.63308
P9-F8	**Collinsella intestinalis**	2.17470	0.00000	97.26683	0.12911
P9-F9	**Collinsella intestinalis**	3.59277	0.00000	96.47777	0.12295
P9-G1	**Collinsella intestinalis**	6.97920	0.00000	95.04295	0.00000
P9-G10	**Peptoniphilus harei**	0.05127	0.00000	4.18809	40.77875
P9-G11	**Collinsella intestinalis**	2.11541	0.00000	96.49217	0.07038
P9-G12	**Collinsella intestinalis**	4.45546	0.00000	95.76433	0.30002
P9-G2	**Collinsella intestinalis**	5.62839	0.00000	94.49581	0.00000
P9-G3	**Collinsella intestinalis**	4.93217	0.05593	96.59442	0.10322
P9-G4	**Collinsella intestinalis**	1.59201	0.00000	97.11176	0.15258
P9-G5	**Collinsella intestinalis**	0.60457	0.00000	97.72769	0.13630
P9-G6	**Collinsella intestinalis**	1.08709	0.00000	97.34953	0.16526
P9-G7	**Collinsella intestinalis**	0.72354	0.00000	95.38806	0.28939
P9-G8	**Collinsella intestinalis**	0.63494	0.00000	92.89789	0.10749
P9-G9	**Collinsella intestinalis**	3.89871	0.00000	96.45528	0.14326
P9-H1	**Anaerococcus rubeinfantis**	0.00000	0.00000	3.25783	0.00000
P9-H10	**Collinsella intestinalis**	4.23827	0.00000	99.60749	0.12120
P9-H11	**Collinsella intestinalis**	2.62418	0.00000	96.81246	0.08107
P9-H12	**Collinsella intestinalis**	12.69548	0.00000	95.72582	0.09783
P9-H2	**Collinsella intestinalis**	2.85363	0.00000	93.15008	0.29110
P9-H3	**Collinsella intestinalis**	2.86053	0.05673	96.41722	0.32567
P9-H4	**Collinsella intestinalis**	1.24102	0.00000	96.04583	0.12649
P9-H5	**Peptoniphilus harei**	0.00000	0.00000	3.42344	50.89230
P9-H6	**Collinsella intestinalis**	#DIV/0!	#DIV/0!	97.23289	0.21211
P9-H7	**Collinsella intestinalis**	2.35148	0.00000	97.70918	0.09586
P9-H8	**Collinsella intestinalis**	0.80755	0.00000	94.58732	0.28606
P9-H9	**Collinsella intestinalis**	2.80643	0.00000	97.22985	0.12701

- PLATE10

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate10	**16S rDNA sequencing**	**3-OxoLCA production (%)**	**isoLCA production (%)**	**LCA production (%)**	**isoLCA production (%)**
P10-A1	**Collinsella intestinalis**	34.13153	0.04609	91.13490	0.10915
P10-A10		0.04946	0.00000	0.00000	3.32532
P10-A11	**Peptoniphilus harei**	0.20042	0.00000	3.45043	43.48243
P10-A12	**Peptoniphilus harei**	0.05607	0.00000	3.29957	48.86068
P10-A2	**Monoglobus pectinilyticus**	2.98334	0.00000	0.22340	0.00000
P10-A3	**Monoglobus pectinilyticus**	2.87063	0.00000	0.04888	0.00000
P10-A4	**Collinsella intestinalis**	27.27120	0.09959	91.05681	0.00000
P10-A5	**Collinsella intestinalis**	0.09288	0.12955	94.76505	0.44230
P10-A6		0.97173	0.00000	0.20248	0.00000
P10-A7		0.09553	0.13916	0.20765	0.00000
P10-A8		0.13614	0.00000	0.19039	0.00000
P10-A9	**Peptoniphilus harei**	20.94046	0.06083	70.95821	17.56274
P10-B1	**Monoglobus pectinilyticus**	2.72237	0.00000	0.10888	0.00000
P10-B10		0.63316	0.30146	0.44183	0.00000
P10-B11	**Collinsella aerofaciens**	0.53360	0.24133	85.19406	0.17345
P10-B12	**Collinsella aerofaciens**	0.37665	0.00000	91.23036	0.32686
P10-B2		0.14864	0.00000	0.00000	0.00000
P10-B3	**Collinsella intestinalis**	33.52895	0.00000	87.06503	0.00000
P10-B4	**Monoglobus pectinilyticus**	1.48688	0.00000	0.00000	0.00000
P10-B5		0.15448	0.00000	0.03048	0.00000
P10-B6	**Collinsella intestinalis**	0.10106	0.18386	86.38025	0.17592
P10-B7	**Collinsella intestinalis**	26.11192	0.00000	86.18871	0.00000
P10-B8	**Collinsella intestinalis**	16.11306	0.88903	86.27787	0.00000
P10-B9		0.13231	0.00000	0.13349	3.05035
P10-C1		0.08269	0.09747	0.04869	0.32269
P10-C2	**Collinsella intestinalis**	8.37484	0.16038	87.09328	0.27866
P10-C3	**Collinsella intestinalis**	6.84692	0.00000	89.59874	0.00000
P10-C4	**Collinsella intestinalis**	29.96992	0.17135	90.76710	0.00000
P10-C5		0.16509	0.00000	0.04407	0.00000
P10-C6		0.07534	0.00000	0.00000	0.00000

- PLATE11

Sequence Summary Report

		LCA as substrate		3-OxoLCA as substrate	
Plate11	16S rDNA sequencing	3-OxoLCA production (%)	isoLCA production (%)	LCA production (%)	isoLCA production (%)
P11-A1	Peptoniphilus harei	0.00000	0.11066	3.66193	45.95645
P11-A10	Collinsella intestinalis	0.86539	0.00000	42.50473	0.13183
P11-A11	Collinsella intestinalis	26.97747	0.00000	83.97298	0.23300
P11-A12	Collinsella intestinalis	46.30576	0.04713	78.00327	0.44037
P11-A2	Peptoniphilus harei	0.06262	0.10561	3.09950	37.90957
P11-A3	Collinsella intestinalis	17.18537	0.06339	51.39268	0.00000
P11-A4	Collinsella intestinalis	0.09696	0.16847	6.02485	0.00000
P11-A5	Peptoniphilus harei	0.00000	0.12610	4.74418	32.36729
P11-A6	Collinsella intestinalis	9.60761	0.22744	89.22872	0.32642
P11-A7	Peptoniphilus harei	0.10321	0.29490	3.10186	39.14505
P11-A8	Peptoniphilus harei	0.22200	0.41791	2.60061	50.62676
P11-A9	Peptoniphilus harei	0.00000	0.10367	3.28555	42.01524
P11-B1	Bacteroides vulgatus	0.00000	0.11906	0.31535	2.95486
P11-B10	Peptoniphilus harei	28.46166	2.75273	69.66825	21.85608
P11-B11	Peptoniphilus harei	0.07911	0.00000	2.92147	42.12848
P11-B12	Peptoniphilus harei	0.00000	0.14852	3.10709	41.23396
P11-B2	Monoglobus pectinilyticus	4.09840	0.00000	0.37248	0.00000
P11-B3	Collinsella intestinalis	42.75195	0.07456	78.54120	0.10154
P11-B4		0.79552	0.00000	0.10954	0.00000
P11-B5		0.06712	0.00000	0.00000	0.00000
P11-B6		0.30473	0.14799	0.00000	0.00000
P11-B7	Peptoniphilus harei	0.11328	0.20032	3.13469	36.07062
P11-B8	Collinsella intestinalis	27.71460	0.08200	78.19122	0.00000
P11-B9	Peptoniphilus harei	0.13525	0.43195	3.38364	41.91333
P11-C1	Collinsella aerofaciens	0.05841	0.00000	91.66464	0.41719
P11-C10		0.08099	0.00000	0.17327	2.06836
P11-C11	Monoglobus pectinilyticus	1.82339	0.12305	0.20410	0.00000
P11-C12	Peptoniphilus harei	0.11067	0.24922	2.11105	28.10889
P11-C2	Collinsella intestinalis	3.48402	0.10618	35.66891	0.00000
P11-C3	Peptoniphilus harei	0.12280	0.15244	2.97525	39.33789
P11-C4	Monoglobus pectinilyticus	0.10822	0.24221	1.27308	0.16743

Sequence Summary Report

P11-C5	**Monoglobus pectinilyticus**	1.19860	0.00000	0.31154	0.08835
P11-C6		0.00000	0.00000	0.00000	0.00000
P11-C7	**Peptoniphilus harei**	0.00000	0.00000	2.68781	34.09251
P11-C8	**Adlercreutzia equolifaciens**	39.81859	0.19673	14.08318	0.00000
P11-C9	**Collinsella intestinalis**	13.59109	0.00000	72.37848	0.00000
P11-D1	**Peptoniphilus harei**	0.06340	0.10766	2.83116	44.82826
P11-D10	**Collinsella intestinalis**	43.42578	0.23388	66.25658	0.17113
P11-D11	**Collinsella intestinalis**	3.57592	0.00000	81.78846	0.00000
P11-D12		0.07987	0.00000	0.06574	0.00000
P11-D2	**Collinsella intestinalis**	8.15272	0.16623	79.53094	0.00000
P11-D3	**Peptoniphilus harei**	0.00000	0.15700	3.81178	48.91274
P11-D4	**Peptoniphilus harei**	0.27014	0.21548	3.09270	42.12123
P11-D5	**Collinsella intestinalis**	13.96320	0.07954	86.93987	0.00000
P11-D6		0.07203	0.13140	0.00000	0.00000
P11-D7	**Collinsella aerofaciens**	0.00000	0.00000	87.14289	0.00000
P11-D8	**Monoglobus pectinilyticus**	1.20169	0.10486	0.06072	0.00000
P11-D9	**Collinsella intestinalis**	5.64109	0.13079	85.44712	0.00000
P11-E1	**Monoglobus pectinilyticus**	3.17484	0.23541	0.08938	0.00000
P11-E10	**Collinsella aerofaciens**	0.11794	0.20400	94.28662	0.21217
P11-E11		0.24904	0.24776	0.07438	0.00000
P11-E12	**Collinsella intestinalis**	38.93470	0.07375	89.41156	0.25841
P11-E2		0.14723	0.00000	0.00000	0.00000
P11-E3		0.00000	0.00000	0.00000	0.00000
P11-E4	**Peptoniphilus harei**	1.22833	0.14916	3.19996	38.01712
P11-E5		0.19518	0.13251	0.25903	0.00000
P11-E6	**Eggerthella lenta**	61.51247	4.68565	44.52899	13.35614
P11-E7	**Collinsella intestinalis**	0.08293	0.08112	84.96732	0.00000
P11-E8	**Monoglobus pectinilyticus**	1.92583	0.00000	0.20726	0.00000
P11-E9	**Peptoniphilus harei**	0.09064	0.00000	2.91248	32.61786
P11-F1	**Monoglobus pectinilyticus**	3.48797	0.00000	0.16052	0.00000
P11-F10	**Peptoniphilus harei**	0.98483	0.00000	2.42459	33.55051
P11-F11	**Collinsella intestinalis**	19.95551	0.00000	91.59552	0.00000
P11-F12	**Monoglobus pectinilyticus**	2.36716	0.00000	1.61500	0.18970
P11-F2	**Peptoniphilus harei**	0.05987	0.00000	4.59756	48.34521
P11-F3	**Peptoniphilus harei**	0.00000	0.23510	2.92159	40.44338
P11-F4	**Peptoniphilus harei**	0.06379	0.00000	3.68128	46.00239
P11-F5		0.07273	0.00000	0.00000	0.00000

Sequence Summary Report

P11-F6	**Peptoniphilus harei**	0.14416	0.00000	2.61786	29.49851
P11-F7	**Peptoniphilus harei**	0.00000	0.09166	4.16206	54.03078
P11-F8	**Peptoniphilus harei**	0.00000	0.11763	3.84235	43.52608
P11-F9	**Peptoniphilus harei**	0.13621	0.12565	3.17480	38.36444
P11-G1		0.21824	0.39175	0.00000	0.00000
P11-G10		0.07388	0.15293	0.69846	0.13031
P11-G11	**Monoglobus pectinilyticus**	1.03655	0.00000	0.36070	0.00000
P11-G12	**Collinsella aerofaciens**	0.27244	0.15139	90.90176	0.27351
P11-G2	**Peptoniphilus harei**	0.06302	0.00000	3.34763	37.33372
P11-G3	**Peptoniphilus harei**	0.00000	0.13599	1.40228	37.46754
P11-G4	**Collinsella intestinalis**	19.45308	0.00000	83.18162	0.37567
P11-G5	**Peptoniphilus harei**	0.00000	0.00000	2.70056	38.32069
P11-G6		0.06538	0.00000	0.00000	0.00000
P11-G7		0.58927	0.00000	0.08500	0.00000
P11-G8		0.71497	0.14668	0.29177	0.00000
P11-G9		0.06738	0.45770	0.19571	3.77796
P11-H1	**Collinsella aerofaciens**	0.06181	0.12437	89.19152	0.23390
P11-H10	**Collinsella intestinalis**	12.48378	0.00000	89.60910	0.00000
P11-H11		0.98537	0.00000	0.88820	0.00000
P11-H12	**Collinsella intestinalis**	2.20309	0.19412	89.71500	0.00000
P11-H2	**Peptoniphilus harei**	0.00000	0.12022	4.13325	45.90040
P11-H3	**Collinsella intestinalis**	26.38131	0.03697	89.88760	0.09504
P11-H4		0.05660	0.23356	0.00000	0.00000
P11-H5	**Peptoniphilus harei**	0.23857	0.46837	2.85276	33.48213
P11-H6	**Peptoniphilus harei**	0.00000	0.16256	1.52549	36.50106
P11-H7	**Collinsella aerofaciens**	0.25774	0.00000	89.80009	0.59266
P11-H8		0.89396	0.18908	0.11399	0.00000
P11-H9	**Peptoniphilus harei**	0.00000	0.00000	3.89692	43.50304

Table S2 - biological triplicate tubes_3-oxoLCA producerss

With 100uM LCA as substrate for 48hr		3-oxoLCA %			isoLCA %		
Human isolates	**16S Sequencing hits**	**Replicate1**	**Replicate2**	**Replicate3**	**Replicate1**	**Replicate2**	**Replicate3**
P4-B10	Phocea massiliensis	2.36	2.47	1.65	0.22	0.51	0.51
P4-F8	Clostridium aldenense	0.84	1.39	1.63	5.10	3.84	3.76
P4-G2	Ruminococcus gnavus	1.15	0.99	1.20	22.36	26.97	32.91
P4-G5	Clostridium perfringens	6.05	7.17	6.61	0.21	0.35	0.18
P7-A2	Raoultibacter massiliensis	47.37	41.59	44.49	0.00	0.00	0.00
P7-E3	Gordonibacter pamelaeae	65.42	69.60	69.47	6.44	4.73	5.25
P7-G1	Collinsella intestinalis	5.12	4.26	4.49	0.00	0.00	0.00
P7-G7	Eggerthella lenta	62.89	62.41	62.20	6.13	6.41	6.04
P8-B9	Monoglobus pectinilyticus	4.14	4.44	3.36	0.60	0.00	0.00
P8-C12	Collinsella intestinalis	22.49	20.35	24.73	0.00	0.00	0.19
P8-F11	Peptoniphilus harei	0.25	0.19	0.00	0.00	0.23	0.00
P2-D12	Phocea massiliensis	0.54	0.39	0.67	0.98	0.10	0.81
P3-E2	Clostridium perfringens	3.27	4.38	4.41	0.00	0.23	0.20
P5-A1	Collinsella aerofaciens	1.26	1.20	0.97	0.00	0.15	0.17
P5-B9	Bifidobacterium longum	1.42	1.65	1.30	0.18	0.17	0.12
P10-A9	Peptoniphilus harei	0.70	0.98	0.87	4.92	5.41	4.87
P11-C8	Adlercreutzia equolifaciens	18.21	15.34	16.36	0.00	0.26	0.12
P11-E6	Eggerthella lenta	19.75	18.69	19.28	34.56	35.86	36.81
P10-A9	Peptoniphilus harei	0.77	1.22	1.66	2.80	1.52	2.89
P11-A12	Collinsella intestinalis	2.05	3.04	2.63	0.13	0.00	0.00
P11-B10	Peptoniphilus harei	0.00	0.00	0.00	0.18	0.00	0.14
P4-G12	Clostridium perfringens	2.03	1.42	1.56	1.03	0.00	0.00
P8-C1	Monoglobus pectinilyticus	0.29	0.24	0.27	0.00	0.00	0.00
P8-C10	Collinsella intestinalis	0.82	1.36	1.52	0.00	0.00	0.00
P10-B8	Collinsella intestinalis	3.66	3.67	3.21	0.00	0.00	0.00
P11-E4	Peptoniphilus harei	0.00	0.07	0.00	0.00	0.00	0.00
P2-B6	Clostridium citroniae	3.75	3.70	3.58	9.50	7.53	8.96
P3-G11	Clostridium perfringens	1.89	2.23	2.45	0.00	0.00	0.00
P5-C2	Collinsella aerofaciens	1.40	1.35	1.05	2.00	2.84	2.17
P5-E12	Bifidobacterium pseudocatenulatum	0.00	0.11	0.00	0.00	0.00	0.00
P5-G3	Bifidobacterium longum	1.82	1.91	1.62	0.21	0.03	0.10
P5-G6	Bifidobacterium longum	1.27	1.61	1.32	0.34	0.00	0.33
P7-G9	Eggerthella lenta	26.68	26.46	25.06	2.79	2.93	2.62
P8-F12	Collinsella intestinalis	4.60	4.55	4.10	0.00	0.00	0.00
P4-B2	Clostridium aldenense	2.99	1.73	2.75	0.83	0.81	1.18

Table S2 - biological triplicate tubes_isoLCA producers

With 100uM 3-oxoLCA as substrate for 48hr		LCA %			isoLCA %		
Human isolates	**16S Sequencing hits**	**Replicate1**	**Replicate2**	**Replicate3**	**Replicate1**	**Replicate2**	**Replicate3**
P4-B10	Phocea massiliensis	99.65	99.70	99.58	0.00	0.00	0.00
P7-E3	Gordonibacter pamelaeae	13.48	22.46	15.64	4.36	8.35	2.71
P7-G7	Eggerthella lenta	15.12	15.59	10.55	3.70	3.94	2.74
P1-B12	Bacteroides dorei	2.70	2.31	2.35	6.08	6.55	5.84
P1-C11	Bacteroides vulgatus	0.96	1.04	0.92	2.60	2.35	2.53
P4-G3	Clostridium perfringens	98.93	98.62	98.75	0.00	0.00	0.00
P5-E1	Bacteroides dorei	3.16	2.30	2.54	6.03	7.09	4.88
P6-C11	Collinsella intestinalis	97.42	96.80	96.80	0.00	0.00	0.00
P6-D1	Bacteroides cellulosilyticus	0.00	0.00	0.00	36.31	40.87	39.92
P6-D2	Collinsella aerofaciens	34.30	31.83	33.76	5.32	2.88	4.65
P6-F10	Bacteroides uniformis	0.00	0.00	0.00	47.84	48.70	44.96
P6-H1	Bacteroides fragilis	0.98	0.85	0.70	44.33	41.04	38.25
P8-G1	Eggerthella lenta	57.16	51.75	51.33	21.66	21.59	23.13
P8-G3	Peptoniphilus harei	4.47	4.09	3.26	74.67	72.87	64.20
P1-A4	Catenibacterium mitsuokai	0.00	0.00	0.00	98.01	95.71	98.98
P1-D2	Bacteroides uniformis	0.00	0.00	0.00	0.00	0.20	0.00
P1-D8	Parabacteroides merdae	0.00	0.00	0.00	6.23	7.98	8.26
P1-F10	Bacteroides uniformis	0.00	0.00	0.00	35.50	36.66	32.20
P1-F2	Bifidobacterium pseudocatenulatum	1.22	1.30	1.03	0.89	0.71	0.62
P1-G2	Bacteroides rodentium	0.00	0.00	0.00	38.63	38.87	38.54
P11-E4	Peptoniphilus harei	6.05	6.28	6.36	75.01	76.11	73.27
P2-A2	Lachnospira pectinoschiza	0.00	0.00	0.00	96.94	96.27	95.15
P2-F2	Lactobacillus rogosae	0.80	0.00	0.00	95.71	94.08	94.31
P3-F8	Ruminococcus gnavus	71.23	71.01	71.48	24.89	24.58	24.11
P3-G11	Clostridium perfringens	97.26	96.87	96.77	0.00	0.00	0.00
P4-A7	Bacillus coagulans	0.00	0.00	0.00	81.26	68.18	51.10
P4-A8	Bacillus coagulans	0.00	0.00	0.00	75.99	78.36	44.35
P5-F6	Collinsella aerofaciens	57.82	54.15	51.63	6.89	10.96	10.63
P5-G11	Bacteroides cellulosilyticus	3.82	5.03	4.02	58.69	65.18	60.39
P6-D10	Bacteroides vulgatus	2.63	2.38	1.80	4.18	4.26	3.15
P6-E4	Collinsella aerofaciens	99.17	99.25	99.68	0.00	0.00	0.00
P6-H1	Bacteroides fragilis	2.28	2.46	3.54	38.88	39.48	40.84
P6-H5	Bacteroides dorei	1.05	1.37	1.32	4.47	4.78	4.65
P7-H12	Peptoniphilus harei	6.38	5.85	5.38	75.73	75.53	74.45
P8-D2	Eggerthella lenta	27.52	30.34	29.29	13.03	15.32	12.06
P8-F11	Peptoniphilus harei	6.00	5.19	4.93	82.94	77.27	78.78
P8-F12	Collinsella intestinalis	92.64	94.06	94.99	0.00	0.00	0.00
P9-B11	Bifidobacterium longum	0.00		0.00	0.00		0.00
P9-D5	Parolsenella catena	0.00	0.00	0.00	0.00	0.00	0.00

Table S2 - biological triplicate tubes_isoLCA producers (continued)

With 100uM 3-oxoLCA as substrate for 48hr		**LCA %**			**isoLCA %**		
Human isolates	**16S Sequencing hits**	**Replicate1**	**Replicate2**	**Replicate3**	**Replicate1**	**Replicate2**	**Replicate3**
P9-D9	Parabacteroides chongii	0.00	0.00	0.00	0.00	0.00	0.00
P4-B2	Clostridium aldenense	21.90	21.26	22.06	6.22	3.14	6.00
P1-A10	Bacteroides fragilis	1.03	0.88	0.88	31.45	30.82	30.50
P4-G2	Ruminococcus gnavus	70.76	70.49	68.18	27.76	27.87	30.32
C.innocuum	Clostridium innocuum DSM1286	0.00	0.00	0.00	90.07	89.14	83.95

*C.innocuum was predicted from bioinformatics listed in **Table S9** - Rumgna_genes_mgx

Supplementary Table 3 | *Bacteroides fragilis* NCTC 9343 3β-HSDH homologs. BLAST alignment of *B. fragilis* NCTC 9343 genome against known 3β-HSDHs Elen_1325 and Rumgna_00694.

	E.lenta **DSM2243 3βHSDH**		***R.gnavus*** **ATCC29149 3βHSDH**	
Insert name	Percent Identity (%)	E-value	Percent Identity	E-value
BF2144	37	4.00E-44	37	6.00E-50
BF3932	35	2.00E-39	31	2.00E-35
BF0083	33	7.00E-35	31	1.00E-31
BF3320	31	5.00E-34	30	7.00E-31
BF1060	32	2.00E-28	30	3.00E-16
BF1669	31	3.00E-24	31	2.00E-21
BF0143	25	7.00E-16	30	4.00E-34
BF2136	26	8.00E-09	-	-
BF3538	28	8.00E-08	-	-
BF2931	25	8.00E-06	31	2.00E-06
BF2345	27	1.00E-05	28	4.00E-07

Genome BLASTed	*B. fragilis* NCTC 9343
Max e-value	1.00E-02
BLAST method	protein vs. protein
MER-FS	Assembled
🟩	expressed and tested

Supplementary table 4 | 3α/3β-HSDH homolog search in *E. lenta* isolates. Presence / absence of Elen_0360, Elen_0690, and Elen_1325 homologs across assayed strains. Locus tags and orthologous group IDs are as reported in ElenMatchR v1.0.9003 [60].

			3α-hydroxysteroid dehydrogenase	**3β-hydroxysteroid dehydrogenase**
Strain Name	**Strain Collection IDs**	**OG_ID30_COV50_2004 (Elen_0360)**	**OG_ID30_COV50_2038 (Elen_0690)**	**OG_ID30_COV50_1765 (Elen_1325)**
Eggerthella lenta 11C	DSM110905	Eggerthella_lenta_11C_00554	Eggerthella_lenta_11C_02552	Eggerthella_lenta_11C_00083
Eggerthella lenta 14A	DSM110907	Eggerthella_lenta_14A_00561	Eggerthella_lenta_14A_02867	Eggerthella_lenta_14A_00168
Eggerthella lenta 22C	DSM110908	Eggerthella_lenta_22C_01352	Eggerthella_lenta_22C_00285	Eggerthella_lenta_22C_00914
Eggerthella lenta 28B	DSM110909	Eggerthella_lenta_28B_02480	Not found	Eggerthella_lenta_28B_00228
Eggerthella lenta A2	DSM110911	Eggerthella_lenta_A2_00417	Eggerthella_lenta_A2_00758	Homolog is split across contigs
Eggerthella lenta DSM 11767	DSM11767	Eggerthella_lenta_DSM11767_02725	Eggerthella_lenta_DSM11767_02379	Eggerthella_lenta_DSM11767_00025
Eggerthella lenta DSM 11863	DSM11863	Eggerthella_lenta_DSM11863_01062	Eggerthella_lenta_DSM11863_00011	Eggerthella_lenta_DSM11863_00792
Eggerthella lenta DSM 15644	DSM15644,ATCC4305,CCUG34779,CIP104211	Eggerthella_lenta_DSM15644_01907	Not found	Eggerthella_lenta_DSM15644_00171
Eggerthella lenta DSM 2243	DSM2243,ATC25559,JCM9979,NCTC11813,VPI0255	Eggerthella_lenta_DSM2243REF_00373	Eggerthella_lenta_DSM2243REF_00704	Eggerthella_lenta_DSM2243REF_01345
Eggerthella lenta FAA 1-1-60AUCSF	DSM110904	Eggerthella_lenta_1160AFAAUCSF_01952	Eggerthella_lenta_1160AFAAUCSF_01137	Eggerthella_lenta_1160AFAAUCSF_00507
Eggerthella lenta FAA 1-3-56	DSM110906	Eggerthella_lenta_1356FAA_01826	Eggerthella_lenta_1356FAA_02297	Eggerthella_lenta_1356FAA_00478
Eggerthella lenta Valencia		Eggerthella_lenta_Valencia_02042	Not found	Eggerthella_lenta_Valencia_00149
Eggerthella sinensis DSM 16107	DSM16107,LMG22123	Eggerthella_sinensis_DSM16107_00168	Eggerthella_sinensis_DSM16107_03005	Eggerthella_sinensis_DSM16107_00947
Gordonibacter pamelaeae 3C	DSM110924	Not found	Gordonibacter_pamelaeae_3C_01808	Gordonibacter_pamelaeae_3C_02959
Gordonibacter species 28C	DSM110925	Not found	Gordonibacter_species_28C_02314	Gordonibacter_species_28C_01887

Supplementary table 5 | 3α/3β-HSDH homolog search in *R. gnavus* isolates. Presence/ absence of Rumgna_02133 (3α-HSDH) and Rumgna_00694 (3β-HSDH) homologs across the assayed strains.

		3α-hydroxysteroid dehydrogenase	**3β-hydroxysteroid dehydrogenase**
Strain_Name	**Assembly accession**	**Locus_tag (Rumgna_02133)**	**Locus_tag (Rumgna_00694)**
[Ruminococcus] gnavus ATCC 35913	GCF_900036035.1	RGNV35913_RS16940	RGNV35913_RS11310
[Ruminococcus] gnavus ATCC 29149	GCF_000169475.1	RUMGNA_02133	RUMGNA_00694
[Ruminococcus] gnavus RJX1118	GCF_002865485.1	Not found	CDL18_06235
[Ruminococcus] gnavus RJX1119	GCF_002865435.1	Not found	CDL22_07295
[Ruminococcus] gnavus RJX1120	GCF_002865405.1	CDL27_01435	CDL27_13985
[Ruminococcus] gnavus RJX1121	GCF_002865465.1	CDL19_03820	CDL19_11930
[Ruminococcus] gnavus RJX1122	GCF_002865425.1	CCY17_11070	CCY17_10550
[Ruminococcus] gnavus RJX1123	GCF_002865355.1	CDL25_02830	CDL25_09750
[Ruminococcus] gnavus RJX1124	GCF_002865325.1	Not found	CDL26_08635
[Ruminococcus] gnavus RJX1125	GCF_002865345.1	Not found	CDL23_04745
[Ruminococcus] gnavus RJX1126	GCF_002865305.1	Not found	CDL24_05470
[Ruminococcus] gnavus RJX1127	GCF_002865385.1	CDL21_08955	CDL21_06950
[Ruminococcus] gnavus RJX1128	GCF_002865285.1	Not found	CDL20_14335

Supplementary Table 6 | Statistical analysis of metabolite differential abundance in the PRISM and HMP2 cohorts based on linear mixed effects models. Nominal p-values were corrected for multiple hypothesis testing using the Benjamini-Hochberg FDR method (yielding adjusted q-values).

- PRISM

Compound	Compound ID	HMDB.ID	Metabolite	prevalence	RT	m.z	coefCD	coefUC	tvalCD	tvalUC	pvalCD	pvalUC	qvalCD	qvalUC
12.63_373.2744m/z_C18-neg	C18-neg_Cluster_0722		3-oxolithocholic acid	0.831168831	12.63	373.2744	-3.051117574	-1.817156482	-2.722486426	-1.524136827	0.007297556	0.129714323	0.039196199	0.295497187
11.73_375.2901m/z_C18-neg	C18-neg_Cluster_0733		isolithocholic acid	0.785714286	11.73	375.2901	-2.666696574	-2.072739042	-2.407205363	-1.758769868	0.017369009	0.080785981	0.070958679	0.226126972
12.42_375.2898m/z_C18-neg	C18-neg_Cluster_0731	HMDB00761	lithocholate	1	12.42	375.2898	-2.018168128	-1.178904823	-2.638771939	-1.448932346	0.009256365	0.149576805	0.045924789	0.321180272
10.89_432.3114m/z_C18-neg	C18-neg_Cluster_1081	HMDB00698	glycolithocholate	0.967532468	10.89	432.3114	-2.438842055	-1.60607758	-2.811996622	-1.740694225	0.005625708	0.083918663	0.032839297	0.231100616
9.51_448.3066m/z_C18-neg	C18-neg_Cluster_1196	HMDB00631	glycodeoxycholate	0.974025974	9.51	448.3066	-1.518289268	-0.267304493	-1.67078337	-0.276501015	0.096982683	0.782568173	0.226814835	0.870923553
10.76_391.2852m/z_C18-neg	C18-neg_Cluster_0833	HMDB00626	deoxycholate	1	10.76	391.2852	-1.373244369	-0.714923024	-2.026957613	-0.991929881	0.044551549	0.322930926	0.134608138	0.508429502
8.54_498.2893m/z_C18-neg	C18-neg_Cluster_1575	HMDB00896	taurodeoxycholate	0.993506494	8.54	498.2893	-0.321925722	-0.080687537	-0.339763864	-0.08004843	0.734539945	0.936312241	0.841569358	0.964156984
9.23_391.2850m/z_C18-neg	C18-neg_Cluster_0830	HMDB00733	hyodeoxycholate/ursodeoxycholate	1	9.23	391.285	-0.198749585	-0.582990758	-0.305481759	-0.842297618	0.760449778	0.401047815	0.859151544	0.582609837
9.70_482.2939m/z_C18-neg	C18-neg_Cluster_1465	HMDB00722	taurolithocholate	0.941558442	9.7	482.2939	0.234693469	0.917648263	0.215130141	0.790681092	0.829976711	0.430458006	0.902423	0.608449872
8.08_448.3067m/z_C18-neg	C18-neg_Cluster_1197	HMDB00708	glycoursodeoxycholate	0.948051948	8.08	448.3067	0.173135415	0.282975358	0.144345529	0.22176392	0.885433739	0.824818531	0.93583355	0.89804924
8.29_498.2890m/z_C18-neg	C18-neg_Cluster_1574	HMDB00951	taurochenodesoxycholate	0.974025974	8.29	498.289	1.105655356	0.630752329	1.191988784	0.639199029	0.235267983	0.523730529	0.410622957	0.684716258
9.26_448.3065m/z_C18-neg		HMDB00637	glycochenodeoxycholate	1	9.26	448.3065	1.057801547	0.425824501	1.439857395	0.544842252	0.152124317	0.586722736	0.307469784	0.733768617
8.12_464.3014m/z_C18-neg		HMDB00138	glycocholate	1	8.12	464.3014	1.157067104	0.465029948	1.373601015	0.518928864	0.171745595	0.604623864	0.333592809	0.746416383
10.55_391.2848m/z_C18-neg	C18-neg_Cluster_0832	HMDB00518	chenodeoxycholate	1	10.55	391.2848	1.631078758	0.555210458	3.455744913	1.105730356	0.000725405	0.270726338	0.008162944	0.455712149
7.38_514.2839m/z_C18-neg		HMDB00036	taurocholate	1	7.38	514.2839	1.941784942	0.947324535	2.025610707	0.928920378	0.044691327	0.354517876	0.134849206	0.540051832
8.10_407.2800m/z_C18-neg	C18-neg_Cluster_0927	HMDB00506	alpha-muricholate	0.993506494	8.1	407.28	2.187165151	0.808464858	2.402343564	0.834717533	0.01759214	0.405288812	0.071594497	0.585766293
8.33_405.2643m/z_C18-neg	C18-neg_Cluster_0900	HMDB00391	ketodeoxycholate	0.993506494	8.33	405.2643	2.371379351	0.893146022	2.900632585	1.026925659	0.004321786	0.306213958	0.027346976	0.49187273
9.11_407.2799m/z_C18-neg	C18-neg_Cluster_0930	HMDB00619	cholate	1	9.11	407.2799	2.30877639	0.867590157	3.963581926	1.400056081	0.000116869	0.163693041	0.002283773	0.337880822
7.26_498.2898m/z_C18-neg	C18-neg_Cluster_1576	HMDB00874	taurohyodeoxycholic acid/tauroursodeoxycholic acid	0.792207792	7.26	498.2898	4.603187682	2.124010486	2.924937788	1.268643086	0.004016146	0.206658841	0.026045119	0.387456826
9.72_391.2852m/z_C18-neg	C18-neg_Cluster_0831		isodeoxycholic acid	1	9.72	391.2852	-1.022070144	-0.891097641	-1.49746267	-1.227228539	0.136508192	0.221781788	0.285791388	0.404565656
10.72_389.2697m/z_C18-neg	C18-neg_Cluster_0818		3-oxodeoxycholic acid	0.993506494	10.72	389.2697	-0.80866379	-0.868133869	-1.29059009	-1.302362488	0.198958117	0.194915806	0.368284884	0.374710369

Table S6 - HMP2

Compound	HMDB ID	Metabolite	RT	m.z	prevalence	coefActiveNonIBD	coefActiveCD	coefActiveUC	tvalActiveNonIBD	tvalActiveCD	tvalActiveUC	pvalActiveNonIBD	pvalActiveCD	pvalActiveUC	qvalActiveNonIBD	qvalActiveCD	qvalActiveUC
C18n_QI6169		3-oxolithocholic acid	12.2	373.2749	0.97985348	-0.60744546	-2.086262023	-2.482534657	-0.774345658	-4.035855028	-2.912574823	0.439252173	6.69E-05	0.003816046	0.816430442	0.00180551	0.316071164
C18n_QI13593		isoallo-lithocholic acid	11.15	751.5889	0.509157509	-3.136617214	-2.793226081	-2.807499558	-2.214795882	-2.962169115	-1.824036278	0.02742134	0.00326481	0.069004054	0.331568822	0.028381117	0.668512129
C18n_QI6230		isolithocholic acid	11.31	375.2906	0.998168498	-0.621043597	-1.944397702	-2.175999246	-0.99048648	-4.629538746	-3.1925764	0.322624575	5.18E-06	0.001538654	0.749582339	0.000278217	0.251447275
C18n_QI48	HMDB00761	lithocholate	11.98	375.2905	1	-0.572602791	-1.750705103	-1.789450074	-1.066461615	-4.856683353	-3.065712017	0.286954329	1.81E-06	0.002341326	0.722670778	0.000127584	0.271011442
C18n_QI55	HMDB00698	glycolithocholate	10.45	432.3119	1	-0.558529916	-1.102496943	-1.624733916	-1.096732885	-3.258664169	-2.935665726	0.273516514	0.001229738	0.003549607	0.712486372	0.014567985	0.312254274
C18n_QI57	HMDB00631	glycodeoxycholate	9.08	448.3074	1	-0.548016241	-0.987318352	-0.984076359	-0.964145592	-2.699955306	-1.593606222	0.335642431	0.007273654	0.111932075	0.756770115	0.049434961	0.735124874
C18n_QI50	HMDB00626	deoxycholate	10.32	391.2857	1	-0.22194394	-1.045715993	-1.54579115	-0.499189364	-3.544349631	-3.199309747	0.617961408	0.000447335	0.001504175	0.894519868	0.007198192	0.250067094
C18n_QI62	HMDB00896	taurodeoxycholate	8.39	498.29	1	-0.876820603	-0.624932091	-1.259852008	-1.22632091	-1.341151152	-1.621924115	0.220907061	0.180746031	0.105725193	0.6659701	0.39271489	0.727955971
C18n_QI51	HMDB00733	hyodeoxycholate/ursodeoxycholate	8.85	391.2855	0.998168498	0.611562243	0.157177606	0.531396148	1.484723235	0.579827832	1.187375523	0.138522375	0.562405922	0.235889367	0.579186679	0.754495436	0.824660967
C18n_QI60	HMDB00722	taurolithocholate	9.65	482.295	1	-0.825346749	-0.626933991	-1.316810359	-1.396949278	-1.601950911	-2.051026051	0.163318971	0.110073749	0.041012761	0.609225428	0.292026026	0.592096945
C18n_QI58	HMDB00708	glycoursodeoxycholate	7.69	448.3071	0.994505495	0.590763639	1.387065804	1.587552352	0.872495392	3.163432312	2.158245667	0.38353977	0.001696487	0.031592219	0.785633186	0.018226509	0.553826924
C18n_QI61	HMDB00951	taurochenodeoxycholate	8.12	498.2899	1	0.534155705	1.946317678	1.241317222	0.774035779	4.390797929	1.655654372	0.439435154	1.50E-05	0.098693263	0.816511526	0.000602642	0.716717188
C18n_QI56	HMDB00637	glycochenodeoxycholate	8.84	448.307	1	0.77033984	1.325585229	0.591029322	1.46272214	3.912140276	1.032979755	0.144445953	0.000110023	0.302330701	0.586076488	0.002596692	0.855063823
C18n_QI59	HMDB00138	glycocholate	7.74	464.3021	1	0.226444234	1.536269431	1.014019547	0.382731019	4.008241791	1.577620284	0.702152869	7.49E-05	0.115561416	0.924570504	0.001957851	0.737744449
C18n_QI49	HMDB00518	chenodeoxycholate	10.12	391.2855	1	0.337056263	1.477807615	1.287355322	0.775761907	5.159392781	2.726936454	0.438416448	4.17E-07	0.006716349	0.815984292	4.21E-05	0.381383737
C18n_QI65	HMDB00036	taurocholate	7.18	514.2845	1	0.245060491	2.017327474	1.487859607	0.366253375	4.624465983	2.046853405	0.714398577	5.30E-06	0.041423224	0.928726976	0.000282505	0.594363113
C18n_QI53	HMDB00506	alpha-muricholate	7.74	407.2804	0.996336996	1.494679417	1.207564188	1.372751672	2.482738741	3.031087096	2.0984038	0.013508416	0.002619327	0.036589923	0.266327585	0.024364032	0.575925564
C18n_QI52	HMDB00391	ketodeoxycholate	7.97	405.2648	1	0.971201619	1.763261605	1.623888453	1.796157506	4.940754434	2.763956034	0.073336715	1.21E-06	0.006014417	0.469223823	9.51E-05	0.366183288
C18n_QI54	HMDB00619	cholate	8.73	407.2804	1	0.444236712	1.676168032	1.488917799	0.94303391	5.387931327	2.908828363	0.346317773	1.32E-07	0.003860957	0.763641529	1.80E-05	0.317225696
C18n_QI63	HMDB00874	taurohyodeoxycholate/tauroursodeoxycholate	7.06	498.29	1	-0.101610082	1.551583707	1.265646526	-0.172858466	4.007115884	1.981634945	0.862863171	7.52E-05	0.048306649	0.97018839	0.00196508	0.61401926
C18n_QI64	HMDB00932	tauro-alpha-muricholate/tauro-beta-muricholate	6.15	514.2844	0.95970696	0.546420194	2.563750376	2.321012033	0.495781415	3.49985466	1.937783584	0.620361586	0.000526015	0.053458322	0.895106098	0.00805811	0.629342019
C18n_QI6769		isodeoxycholic acid	9.31	391.2858	1	0.025287813	-0.879409103	-1.130266744	0.060391028	-3.20380616	-2.484472406	0.95187887	0.00148155	0.013443986	0.991905926	0.016592322	0.451248618
C18n_QI6700		3-oxodeoxycholic acid	10.28	389.2703	1	0.129492557	0.314102878	-0.642858366	0.37122224	1.363903475	-1.69606246	0.710697904	0.173479459	0.090768368	0.927365458	0.383159277	0.705949302

Supplementary Table 7 | TH17/IL-17a-related genes used in this study. We collected TH17/IL-17α-related genes including a group of genes enriched in the IL-17 signaling pathway[6] and another group of TH17 signature genes found by Revu et al[7].

gene	host	reference
CCL2	Human	[61]
CCL11	Human	[61]
CCL20	Human	[61]
CXCL1	Human	[61]
CXCL2	Human	[61]
CXCL3	Human	[61]
CXCL5	Human	[61]
CXCL6	Human	[61]
CXCL10	Human	[61]
DEFB4A	Human	[61]
IFNG	Human	[61]
IL1B	Human	[61]
IL6	Human	[61]
IL17A	Human	[61]
LCN2	Human	[61]
MMP1	Human	[61]
MMP3	Human	[61]
MMP9	Human	[61]
MMP13	Human	[61]
MUC5AC	Human	[61]
TNF	Human	[61]
RORC	Human	[62]
IL17A	Human	[62]
IL17F	Human	[62]
IL26	Human	[62]
GZMA	Human	[62]
GZMB	Human	[62]
CXCL13	Human	[62]
CCR6	Human	[62]
IL23R	Human	[62]
IL1R1	Human	[62]
IL6R	Human	[62]
IL6ST	Human	[62]
TCF7	Human	[62]
LEF1	Human	[62]
BATF	Human	[62]
MAF	Human	[62]
JUN	Human	[62]
JUNB	Human	[62]
JUND	Human	[62]
FOS	Human	[62]

Table S7 (continued)

FOSL2	Human	[62]
BCL-XL	Human	[62]
BCL6	Human	[62]
IL2	Human	[62]
IL2RA	Human	[62]
OSM	Human	[62]
SOCS3	Human	[62]
GFI1	Human	[62]
FOXP3	Human	[62]
CTLA4	Human	[62]
LAG3	Human	[62]
PD1	Human	[62]
IL21	Human	[62]
CXCR5	Human	[62]
ICOS	Human	[62]
IL22	Human	[62]

Supplementary Table 8 | Differential expression modeling of TH17/IL-17α-related genesin HMP2. Table fields indicate 1) gene name; 2) condition (i.e. CD:Non-IBD and UC:Non-IBD); 3) effect size estimated from the linear model's diagnosis coefficient; 4) nominal p-values from the linear models (**Methods**); 5) adjusted p-values based on the Benjamini-Hochberg procedure with target false discovery rate (FDR) of 0.25.

gene	**condition**	***effect size**	***p*-value**	***q*-value**
BATF	CD_vs_nonIBD	0.66565954	0.0832764	0.3825344
BATF	UC_vs_nonIBD	0.47592211	0.25372625	0.75758555
BCL6	CD_vs_nonIBD	0.2382921	0.42731984	0.75283582
BCL6	UC_vs_nonIBD	-0.0618586	0.84998722	0.96238886
CCL11	CD_vs_nonIBD	1.61334959	0.0049228	0.1225743
CCL11	UC_vs_nonIBD	2.16071217	0.00067176	0.544394
CCL2	CD_vs_nonIBD	1.14045415	0.00146368	0.07581674
CCL2	UC_vs_nonIBD	0.69496116	0.06839691	0.67073598
CCL20	CD_vs_nonIBD	1.25406623	0.02053657	0.21877253
CCL20	UC_vs_nonIBD	0.22469294	0.69826699	0.91934478
CCR6	CD_vs_nonIBD	0.58705187	0.22486062	0.58186804
CCR6	UC_vs_nonIBD	0.56940436	0.28042483	0.76823466
CTLA4	CD_vs_nonIBD	0.92062258	0.05297442	0.31656802
CTLA4	UC_vs_nonIBD	0.72813153	0.15824584	0.71702747
CXCL1	CD_vs_nonIBD	2.59536684	6.60E-05	0.0249417
CXCL1	UC_vs_nonIBD	1.31474778	0.05240926	0.66118259
CXCL10	CD_vs_nonIBD	2.11897054	6.72E-05	0.0249417
CXCL10	UC_vs_nonIBD	0.44831128	0.41297844	0.82083204
CXCL13	CD_vs_nonIBD	-0.7948318	0.42144955	0.74813925
CXCL13	UC_vs_nonIBD	-0.727229	0.50024863	0.85092407
CXCL2	CD_vs_nonIBD	1.97153759	0.00164748	0.07966999
CXCL2	UC_vs_nonIBD	0.46483351	0.48121401	0.84327297
CXCL3	CD_vs_nonIBD	2.01392878	0.00251582	0.09752794
CXCL3	UC_vs_nonIBD	0.78341499	0.26733981	0.76421472
CXCL5	CD_vs_nonIBD	3.50329909	7.12E-05	0.0249417
CXCL5	UC_vs_nonIBD	1.8847253	0.04072925	0.64174526
CXCL6	CD_vs_nonIBD	2.44953922	2.03E-05	0.01542235
CXCL6	UC_vs_nonIBD	1.39610444	0.0194653	0.61892197
CXCR5	CD_vs_nonIBD	-0.5195156	0.48335088	0.78780195
CXCR5	UC_vs_nonIBD	-0.3038025	0.70701093	0.92221105
DEFB4A	CD_vs_nonIBD	2.49965596	0.0101783	0.16390778
DEFB4A	UC_vs_nonIBD	1.63524631	0.11780651	0.69451674
FOS	CD_vs_nonIBD	0.30656161	0.47545646	0.7834018
FOS	UC_vs_nonIBD	0.28562745	0.54236613	0.86507241
FOSL2	CD_vs_nonIBD	0.03764232	0.74903629	0.91611769
FOSL2	UC_vs_nonIBD	-0.1049566	0.41497136	0.82126252
FOXP3	CD_vs_nonIBD	0.88351876	0.04632224	0.30033775
FOXP3	UC_vs_nonIBD	0.7314862	0.12845262	0.70114245
GFI1	CD_vs_nonIBD	-0.0469246	0.64657473	0.8736897
GFI1	UC_vs_nonIBD	0.04423487	0.69215384	0.91742631
GZMA	CD_vs_nonIBD	0.41631414	0.14528505	0.48601648

Table S8 (continued)

GZMA	UC_vs_nonIBD	0.24585154	0.42830192	0.82734642
GZMB	CD_vs_nonIBD	2.0712882	1.45E-05	0.0138762
GZMB	UC_vs_nonIBD	0.96043774	0.05101453	0.65633306
ICOS	CD_vs_nonIBD	0.67927459	0.07568473	0.36633229
ICOS	UC_vs_nonIBD	0.68415145	0.10073633	0.6926757
IFNG	CD_vs_nonIBD	2.14467674	0.00021539	0.03418664
IFNG	UC_vs_nonIBD	1.35779491	0.02649308	0.62423699
IL17A	CD_vs_nonIBD	2.5119816	0.00024102	0.03617232
IL17A	UC_vs_nonIBD	1.31400284	0.06745852	0.66897715
IL17F	CD_vs_nonIBD	1.5004707	0.00773224	0.14643648
IL17F	UC_vs_nonIBD	0.27859696	0.64202275	0.90085366
IL1B	CD_vs_nonIBD	2.43670028	6.88E-05	0.0249417
IL1B	UC_vs_nonIBD	0.73837514	0.2429393	0.75120037
IL1R1	CD_vs_nonIBD	0.64263058	0.00982924	0.16230729
IL1R1	UC_vs_nonIBD	0.48776957	0.06910566	0.67133823
IL2	CD_vs_nonIBD	0.38557979	0.33467547	0.68342041
IL2	UC_vs_nonIBD	0.39172329	0.36917548	0.80287802
IL21	CD_vs_nonIBD	0.41709149	0.50180211	0.79823766
IL21	UC_vs_nonIBD	0.55030783	0.4173966	0.82217495
IL22	CD_vs_nonIBD	2.49564249	0.00015701	0.03033808
IL22	UC_vs_nonIBD	0.91028228	0.18528717	0.73205688
IL23R	CD_vs_nonIBD	-0.0800676	0.69881493	0.89620542
IL23R	UC_vs_nonIBD	-0.2096058	0.35487654	0.80015574
IL26	CD_vs_nonIBD	2.32519973	2.82E-05	0.01684496
IL26	UC_vs_nonIBD	1.52221211	0.0088761	0.59963935
IL2RA	CD_vs_nonIBD	1.13797108	0.00686762	0.13905217
IL2RA	UC_vs_nonIBD	0.77523553	0.0863925	0.68533727
IL6	CD_vs_nonIBD	1.92724443	0.00254056	0.09752794
IL6	UC_vs_nonIBD	0.35941129	0.59396285	0.88580386
IL6R	CD_vs_nonIBD	-0.1221817	0.33898405	0.68657973
IL6R	UC_vs_nonIBD	-0.2360782	0.0929874	0.68618118
IL6ST	CD_vs_nonIBD	0.25539572	0.08590989	0.38841833
IL6ST	UC_vs_nonIBD	0.25076081	0.12174327	0.69451674
JUN	CD_vs_nonIBD	-0.3127255	0.12800662	0.45920034
JUN	UC_vs_nonIBD	-0.4123252	0.06715476	0.66897715
JUNB	CD_vs_nonIBD	0.142444	0.624793	0.86285372
JUNB	UC_vs_nonIBD	-0.1910048	0.54829593	0.86708588
JUND	CD_vs_nonIBD	-0.1804596	0.26474693	0.62220295
JUND	UC_vs_nonIBD	-0.0224416	0.89846453	0.97534441
LAG3	CD_vs_nonIBD	0.75072333	0.00353271	0.11068579
LAG3	UC_vs_nonIBD	0.84006144	0.00283684	0.58005734
LCN2	CD_vs_nonIBD	1.99882921	0.00621587	0.13483987
LCN2	UC_vs_nonIBD	0.80038912	0.30386257	0.77779511

Table S8 (continued)

LEF1	CD_vs_nonIBD	0.21464072	0.56904538	0.83350678
LEF1	UC_vs_nonIBD	0.47128625	0.25391462	0.7576485
MAF	CD_vs_nonIBD	0.090307	0.84436383	0.95422368
MAF	UC_vs_nonIBD	0.60468103	0.23110106	0.74722093
MMP1	CD_vs_nonIBD	2.75410459	0.00074791	0.0589297
MMP1	UC_vs_nonIBD	1.43742136	0.09586379	0.69047639
MMP13	CD_vs_nonIBD	2.59811573	0.00049254	0.04894808
MMP13	UC_vs_nonIBD	0.84126055	0.28121054	0.76831517
MMP3	CD_vs_nonIBD	3.72374924	1.00E-04	0.02560496
MMP3	UC_vs_nonIBD	2.19330868	0.02895379	0.62423699
MMP9	CD_vs_nonIBD	0.51876709	0.22250504	0.57976923
MMP9	UC_vs_nonIBD	0.9222929	0.04902445	0.65510444
MUC5AC	CD_vs_nonIBD	0.83868511	0.24737376	0.60565531
MUC5AC	UC_vs_nonIBD	0.40275613	0.6094913	0.89067144
OSM	CD_vs_nonIBD	2.88265035	0.00013296	0.02793591
OSM	UC_vs_nonIBD	1.10084449	0.16073828	0.71829205
RORC	CD_vs_nonIBD	-0.5521908	0.00327323	0.1081523
RORC	UC_vs_nonIBD	-0.4316474	0.03249	0.62423699
SOCS3	CD_vs_nonIBD	2.04467339	2.34E-05	0.01616636
SOCS3	UC_vs_nonIBD	0.93418108	0.0614125	0.66644493
TCF7	CD_vs_nonIBD	0.14508972	0.6346556	0.86771627
TCF7	UC_vs_nonIBD	0.47570566	0.15640088	0.71454055
TNF	CD_vs_nonIBD	0.88193266	0.01994997	0.21628315
TNF	UC_vs_nonIBD	0.54404506	0.18251773	0.72969256

[*] The effect size is represented by the estimated coefficient from the linear model. Positive value means that genes are up-regulated in IBD (CD or UC) compared to Non-IBD condition. Negetive value means down-regulated cases.

Supplementary Table 9 | Differential abundance modeling of 3α- and 3β-HSDH homologs in HMP2. Table fields in the first sheet indicate 1) homolog ID; 2) class (i.e. 3α-HSDH-based homolog and 3β-HSDH based homolog); 3-7) the prevalence of each homolog in each disease phenotype; 8-9) effect size estimated from the linear model's dysbiosis coefficient; 10-11) nominal p-values from the linear mixed-effects models (**Methods**); and 12-13) adjusted p-values based on the Benjamini-Hochberg procedure with target false discovery rate (FDR) of 0.05. Table fields in the 2-4 sheets follow the same format as the first sheet except the first three fields: 1) the UniRef90 annotations (which had been pre-computed using HUMAnN) (i.e. protein sequences with >90% amino acid identity and >80% coverage) of the genes identified as 3α- and/ or 3β-HSDHs; 2) the genes identified as 3α- and/ or 3β-HSDHs (Elen_1325 and Elen_0690 from E. lenta; Rumgna_02133 and Rumgna_00694 from R. gnavus; BF3538 from B. fragilis NCTC 9343); 3) the homolog of a given UniRef90 - the UniRef50 family (i.e. a set of proteins expected to have >50% identity and high coverage of the query) including all UniRef90 families belonging to it.

- sum_mgx

Homolog ID	class	pre.CD-dys	pre.CD-nondys	pre.UC-dys	pre.UC-nondys	prev.nonIBD-nondys	coef.CD-dys	coef.UC-dys	pval.CD-dys	pval.UC-dys	qval.CD-dys	qval.UC-dys
3aHSDH	3aHSDH	0.81920904	0.990990991	0.921568627	0.989637306	0.997389034	-0.655616711	-0.3446491	9.32E-25	7.72E-05	6.52E-24	0.000199341
Rumgna_02133 homolog	3aHSDH	0.807909605	0.987387387	0.921568627	0.989637306	0.997389034	-0.666843011	-0.357198708	9.61E-24	8.54E-05	3.36E-23	0.000199341
Elen_0690 homolog	3aHSDH	0.237288136	0.598198198	0.509803922	0.621761658	0.72845953	-0.346298054	-0.187409185	5.29E-05	0.107944832	0.000123515	0.151122764
3bHSDH	3bHSDH	0.700564972	0.637837838	0.607843137	0.60880829	0.514360313	-0.101283607	-0.433158446	0.278365728	0.000459439	0.31886309	0.000804018
BF3538 homolog	3bHSDH	0.355932203	0.466666667	0.392156863	0.409326425	0.318537859	-0.15905823	-0.439106202	0.031893425	6.94E-06	0.055813494	4.86E-05
Elen_1325 homolog	3bHSDH	0.333333333	0.174774775	0.215686275	0.186528497	0.161879896	0.108491423	-0.040712517	0.056796773	0.600118774	0.079515483	0.600118774
Rumgna_00694 homolog	3bHSDH	0.242937853	0.216216216	0.156862745	0.233160622	0.187989556	0.055924554	-0.057733265	0.31886309	0.457082572	0.31886309	0.533263001

Table S9 - Elen_genes_mgx

HUMAnN2 Homolog + Stratification	Query Gene ID	Query UniRef50	pre.CD-dys	pre.CD-nondys	pre.UC-dys	pre.UC-nondys	prev.nonIBD-nondys	coef.CD-dys	coef.UC-dys	pval.CD-dys	pval.UC-dys	qval.CD-dys	qval.UC-dys
UniRef90_C4Z6X3	ELEN_0690	UniRef50_R5H8Q8	0.1469	0.5117	0.3529	0.5699	0.6710	-0.2372	-0.2852	0.0005	0.0021	0.0067	0.0103
UniRef90_C4Z6X3|unclassified	ELEN_0690	UniRef50_R5H8Q8	0.1469	0.5117	0.3529	0.5699	0.6710	-0.2372	-0.2852	0.0005	0.0021	0.0067	0.0103
UniRef90_R7R433	ELEN_0690	UniRef50_R5H8Q8	0.0339	0.0523	0.0588	0.0751	0.1697	-0.0289	-0.0040	0.3448	0.9282	0.7869	0.9953
UniRef90_R7R433|unclassified	ELEN_0690	UniRef50_R5H8Q8	0.0339	0.0523	0.0588	0.0751	0.1697	-0.0289	-0.0040	0.3448	0.9282	0.7869	0.9953
UniRef90_R5IF04	ELEN_0690	UniRef50_R5H8Q8	0.0282	0.0865	0.0784	0.0829	0.0992	-0.0229	0.0442	0.4161	0.2490	0.7869	0.7782
UniRef90_R5IF04|unclassified	ELEN_0690	UniRef50_R5H8Q8	0.0282	0.0865	0.0784	0.0829	0.0992	-0.0229	0.0442	0.4161	0.2490	0.7869	0.7782
UniRef90_C8WMP0|unclassified	ELEN_0690	UniRef50_R5H8Q8	0.0000	0.0018	0.0000	0.0000	0.0052	-0.0012	-0.0001	0.5292	0.9762	0.8268	0.9953
UniRef90_C8WMP0|g__Gordonibacter|s__Gordonibacter_p	ELEN_0690	UniRef50_R5H8Q8	0.0000	0.0000	0.0000	0.0078	0.0052	-0.0011	-0.0045	0.7532	0.4616	0.9953	0.9331
UniRef90_R7BJD8	ELEN_0690	UniRef50_R5H8Q8	0.0000	0.0000	0.0588	0.0052	0.0444	-0.0006	0.0791	0.9555	0.0000	0.9953	0.0000
UniRef90_R7BJD8|unclassified	ELEN_0690	UniRef50_R5H8Q8	0.0000	0.0000	0.0588	0.0052	0.0444	-0.0006	0.0791	0.9555	0.0000	0.9953	0.0000
UniRef90_R5U0E4|unclassified	ELEN_1325	UniRef50_C8WGQ3	0.0000	0.0018	0.0000	0.0000	0.0000	-0.0005	0.0000	0.4721	0.9878	0.7869	0.9953
UniRef90_C8WGQ3|unclassified	ELEN_1325	UniRef50_C8WGQ3	0.0000	0.0018	0.0000	0.0000	0.0000	-0.0005	0.0000	0.4713	0.9953	0.7869	0.9953
UniRef90_C8WMP0|g__Peptostreptococcaceae_noname|s_	ELEN_0690	UniRef50_R5H8Q8	0.0000	0.0000	0.0196	0.0000	0.0000	0.0000	0.0060	0.9977	0.0000	0.9977	0.0000
UniRef90_C8WGQ3|g__Gordonibacter|s__Gordonibacter_p	ELEN_1325	UniRef50_C8WGQ3	0.0056	0.0000	0.0000	0.0104	0.0052	0.0005	-0.0083	0.9272	0.3201	0.9953	0.8893
UniRef90_R5H8Q8	ELEN_0690	UniRef50_R5H8Q8	0.0056	0.0108	0.0196	0.0181	0.0183	0.0013	-0.0107	0.9005	0.4742	0.9953	0.9331
UniRef90_R5H8Q8|unclassified	ELEN_0690	UniRef50_R5H8Q8	0.0056	0.0108	0.0196	0.0181	0.0183	0.0013	-0.0107	0.9005	0.4742	0.9953	0.9331
UniRef90_C8WGQ3|g__Peptostreptococcaceae_noname|s_	ELEN_1325	UniRef50_C8WGQ3	0.0056	0.0000	0.0196	0.0026	0.0000	0.0020	0.0072	0.4170	0.0674	0.7869	0.2807
UniRef90_A6NSX2	ELEN_0690	UniRef50_R5H8Q8	0.0282	0.0360	0.0784	0.0492	0.0548	0.0030	-0.0059	0.8865	0.8482	0.9953	0.9953
UniRef90_A6NSX2|g__Pseudoflavonifractor|s__Pseudoflavo	ELEN_0690	UniRef50_R5H8Q8	0.0282	0.0360	0.0784	0.0492	0.0548	0.0030	-0.0059	0.8865	0.8482	0.9953	0.9953
UniRef90_C8WMP0	ELEN_0690	UniRef50_R5H8Q8	0.0395	0.0108	0.0196	0.0078	0.0078	0.0087	0.0108	0.3970	0.4852	0.7869	0.9331
UniRef90_C8WMP0|g__Eggerthella|s__Eggerthella_lenta	ELEN_0690	UniRef50_R5H8Q8	0.0395	0.0090	0.0000	0.0000	0.0026	0.0094	0.0004	0.2318	0.9707	0.7869	0.9953
UniRef90_C8WGQ3|g__Eggerthella|s__Eggerthella_lenta	ELEN_1325	UniRef50_C8WGQ3	0.0508	0.0072	0.0000	0.0052	0.0026	0.0116	-0.0048	0.0928	0.6292	0.3868	0.9953
UniRef90_C8WGQ3	ELEN_1325	UniRef50_C8WGQ3	0.0621	0.0090	0.0196	0.0181	0.0078	0.0244	-0.0088	0.0354	0.6145	0.2948	0.9953
UniRef90_R5U0E4	ELEN_1325	UniRef50_C8WGQ3	0.3164	0.1694	0.2157	0.1813	0.1567	0.1042	-0.0265	0.0632	0.7286	0.3161	0.9953
UniRef90_R5U0E4|g__Clostridium|s__Clostridium_hathewa	ELEN_1325	UniRef50_C8WGQ3	0.3164	0.1676	0.2157	0.1813	0.1567	0.1047	-0.0268	0.0614	0.7253	0.3161	0.9953

Table S9 - Rumgna_genes_mgx

HUMAnN2 Homolog + Stratification	Query Gene ID	Query UniRef50	pre.CD-dys	pre.CD-nondys	pre.UC-dys	pre.UC-nondys	prev.nonIBD-nondys	coef.CD-dys	coef.UC-dys	pval.CD-dys	pval.UC-dys	qval.CD-dys	qval.UC-dys
UniRef90_D4LGZ3	Rumgna_02133	UniRef50_R5B9W8	0.5989	0.9766	0.9020	0.9819	0.9922	-0.8349	-0.4206	0.0000	0.0000	0.0000	0.0038
UniRef90_D4LGZ3|g__Roseburia|s__Roseburia_inulinivorans	Rumgna_02133	UniRef50_R5B9W8	0.2599	0.5730	0.4706	0.7073	0.7963	-0.7154	-0.0522	0.0000	0.6734	0.0000	0.9993
UniRef90_D4LGZ3|g__Eubacterium|s__Eubacterium_rectale	Rumgna_02133	UniRef50_R5B9W8	0.2599	0.6306	0.3333	0.6218	0.7415	-0.6060	-0.4550	0.0000	0.0014	0.0000	0.0700
UniRef90_D4LGZ3|g__Blautia|s__Ruminococcus_obeum	Rumgna_02133	UniRef50_R5B9W8	0.2881	0.8108	0.7059	0.7953	0.8773	-0.4845	-0.2470	0.0000	0.0261	0.0000	0.2179
UniRef90_D4LGZ3|g__Dorea|s__Dorea_formicigenerans	Rumgna_02133	UniRef50_R5B9W8	0.0565	0.4919	0.4706	0.6528	0.6945	-0.3700	-0.2329	0.0000	0.0299	0.0000	0.2223
UniRef90_D7GRT2	Rumgna_02133	UniRef50_R5B9W8	0.2542	0.5009	0.3725	0.5233	0.6136	-0.3348	-0.2855	0.0000	0.0096	0.0004	0.1360
UniRef90_D7GRT2|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.2542	0.5009	0.3725	0.5233	0.6136	-0.3348	-0.2855	0.0000	0.0096	0.0004	0.1360
UniRef90_D4LGZ3|g__Eubacterium|s__Eubacterium_hallii	Rumgna_02133	UniRef50_R5B9W8	0.1356	0.3910	0.2353	0.5440	0.5614	-0.2458	-0.2837	0.0006	0.0044	0.0036	0.1137
UniRef90_D4LGZ3|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.2090	0.4180	0.2549	0.3938	0.4778	-0.2412	-0.1718	0.0002	0.0619	0.0014	0.3576
UniRef90_D4LGZ3|g__Ruminococcus|s__Ruminococcus_lactaris	Rumgna_02133	UniRef50_R5B9W8	0.0791	0.1892	0.0392	0.3523	0.3995	-0.1780	-0.1159	0.0019	0.1237	0.0100	0.5362
UniRef90_U2C7T4|g__Clostridium|s__Clostridium_sp_KLE_1755	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0721	0.0784	0.0466	0.0052	-0.0947	-0.0063	0.0064	0.8934	0.0263	0.9993
UniRef90_A4E7X7	Rumgna_02133	UniRef50_R5B9W8	0.0565	0.2739	0.1765	0.3705	0.2924	-0.0940	-0.1121	0.0771	0.1165	0.2430	0.5267
UniRef90_A4E7X7|g__Collinsella|s__Collinsella_aerofaciens	Rumgna_02133	UniRef50_R5B9W8	0.0565	0.2703	0.1765	0.3705	0.2924	-0.0865	-0.0996	0.0934	0.1502	0.2775	0.6247
UniRef90_R6BIQ6	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0685	0.0000	0.0104	0.0914	-0.0762	-0.0037	0.0051	0.9228	0.0219	0.9993
UniRef90_R6BIQ6|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0685	0.0000	0.0104	0.0914	-0.0762	-0.0037	0.0051	0.9228	0.0219	0.9993
UniRef90_B9Y5C1|g__Holdemania|s__Holdemania_filiformis	Rumgna_00694	UniRef50_R5TQC2	0.0904	0.1892	0.0588	0.2124	0.1671	-0.0662	-0.1525	0.1740	0.0259	0.4413	0.2179
UniRef90_B9Y5C1	Rumgna_00694	UniRef50_R5TQC2	0.1017	0.1892	0.0588	0.2124	0.1697	-0.0460	-0.1523	0.3491	0.0272	0.7892	0.2179
UniRef90_R5TKT5|g__Lachnospiraceae_noname|s__Lachnospiraceae_bacterium_2_1_58FAA	Rumgna_02133	UniRef50_R5B9W8	0.1186	0.0793	0.1373	0.0777	0.0627	-0.0451	-0.0076	0.1976	0.8772	0.4892	0.9993
UniRef90_D4LGZ3|g__Ruminococcus|s__Ruminococcus_sp_5_1_39BFAA	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0793	0.0196	0.0777	0.1070	-0.0386	-0.1468	0.3862	0.0246	0.8313	0.2179
UniRef90_C4FBF0	Rumgna_02133	UniRef50_R5B9W8	0.0226	0.0450	0.1176	0.0829	0.0183	-0.0356	-0.0715	0.1666	0.0396	0.4332	0.2577
UniRef90_C4FBF0|g__Collinsella|s__Collinsella_intestinalis	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0234	0.1176	0.0622	0.0104	-0.0325	-0.0674	0.0977	0.0105	0.2821	0.1360
UniRef90_R5BAL7	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0252	0.0000	0.0026	0.0313	-0.0295	0.0000	0.0285	0.9993	0.0927	0.9993
UniRef90_R5BAL7|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0252	0.0000	0.0026	0.0313	-0.0295	0.0000	0.0285	0.9993	0.0927	0.9993
UniRef90_U5F5L7|g__Eubacterium|s__Eubacterium_sp_3_1_31	Rumgna_02133	UniRef50_R5B9W8	0.0791	0.0613	0.0980	0.0518	0.0653	-0.0237	0.0128	0.4858	0.7793	0.9294	0.9993
UniRef90_R6WN40	Rumgna_02133	UniRef50_R5B9W8	0.0226	0.0306	0.0196	0.0207	0.0444	-0.0229	0.0031	0.1529	0.8881	0.4078	0.9993
UniRef90_R6WN40|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0226	0.0306	0.0196	0.0207	0.0444	-0.0229	0.0031	0.1529	0.8881	0.4078	0.9993
UniRef90_A4E7X7|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0324	0.0000	0.0544	0.0209	-0.0209	-0.0723	0.2783	0.0075	0.6731	0.1360
UniRef90_R6NVR4	Rumgna_02133	UniRef50_R5B9W8	0.0113	0.0378	0.0588	0.0622	0.0392	-0.0114	0.0062	0.5487	0.8182	0.9746	0.9993
UniRef90_R6NVR4|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0113	0.0378	0.0588	0.0622	0.0392	-0.0114	0.0062	0.5487	0.8182	0.9746	0.9993
UniRef90_S6CFR4	Rumgna_02133	UniRef50_R5B9W8	0.0113	0.0144	0.0000	0.0207	0.0809	-0.0103	-0.0154	0.5904	0.5870	0.9746	0.9993
UniRef90_S6CFR4|g__Adlercreutzia|s__Adlercreutzia_equolifaciens	Rumgna_02133	UniRef50_R5B9W8	0.0113	0.0144	0.0000	0.0207	0.0809	-0.0103	-0.0154	0.5904	0.5870	0.9746	0.9993
UniRef90_E7GCZ0	Rumgna_02133	UniRef50_R5B9W8	0.0113	0.0198	0.0000	0.0078	0.0183	-0.0074	-0.0080	0.5334	0.6779	0.9746	0.9993
UniRef90_R5QVC4	Rumgna_02133	UniRef50_R5B9W8	0.0226	0.0306	0.0392	0.0130	0.0235	-0.0066	0.0031	0.6753	0.8982	0.9851	0.9993
UniRef90_R5QVC4|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0226	0.0306	0.0392	0.0130	0.0235	-0.0066	0.0031	0.6753	0.8982	0.9851	0.9993
UniRef90_R7NJY1	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0198	0.0000	0.0130	0.0104	-0.0048	-0.0291	0.7418	0.2075	0.9851	0.7992
UniRef90_R7NJY1|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0198	0.0000	0.0130	0.0104	-0.0048	-0.0291	0.7418	0.2075	0.9851	0.7992
UniRef90_E7GCZ0|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0090	0.0000	0.0052	0.0078	-0.0039	-0.0048	0.5771	0.6584	0.9746	0.9993
UniRef90_R9IUF6	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0162	0.0000	0.0104	0.0131	-0.0036	-0.0101	0.7316	0.5422	0.9851	0.9993
UniRef90_R9IUF6|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0169	0.0162	0.0000	0.0104	0.0131	-0.0036	-0.0101	0.7316	0.5422	0.9851	0.9993
UniRef90_R7AYJ2	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0233	0.0078	-0.0031	-0.0189	0.6814	0.0816	0.9851	0.4241
UniRef90_R7AYJ2|g__Erysipelotrichaceae_noname|s__Eubacterium_cylindroides	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0233	0.0078	-0.0031	-0.0189	0.6814	0.0816	0.9851	0.4241
UniRef90_C4FBF0|g__Collinsella|s__Collinsella_tanakaei	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0216	0.0000	0.0155	0.0078	-0.0027	-0.0005	0.8410	0.9768	0.9851	0.9993
UniRef90_R5B9W8	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0144	0.0000	0.0000	0.0026	-0.0021	0.0013	0.6974	0.8663	0.9851	0.9993
UniRef90_R5B9W8|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0144	0.0000	0.0000	0.0026	-0.0021	0.0013	0.6974	0.8663	0.9851	0.9993
UniRef90_E7GCZ0|g__Coprobacillus|s__Coprobacillus_sp_D6	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0036	0.0000	0.0000	0.0052	-0.0017	-0.0001	0.5999	0.9896	0.9749	0.9993
UniRef90_E7GCZ0|g__Coprobacillus|s__Coprobacillus_sp_29_1	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0090	0.0000	0.0026	0.0078	-0.0014	-0.0020	0.8474	0.8679	0.9851	0.9993
UniRef90_R7GA34	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0018	0.0000	0.0052	0.0235	-0.0011	-0.0016	0.8834	0.8895	0.9851	0.9993
UniRef90_R7GA34|g__Erysipelotrichaceae_noname|s__Eubacterium_dolichum	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0018	0.0000	0.0052	0.0235	-0.0011	-0.0016	0.8834	0.8895	0.9851	0.9993
UniRef90_R7B6R4	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0000	0.0104	-0.0009	0.0004	0.8845	0.9668	0.9851	0.9993
UniRef90_R7B6R4|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0000	0.0104	-0.0009	0.0004	0.8845	0.9668	0.9851	0.9993
UniRef90_D4LGZ3|g__Clostridium|s__Clostridium_sp_L2_50	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0054	0.0000	0.0052	0.0078	-0.0007	-0.0070	0.8701	0.2590	0.9851	0.8980
UniRef90_R5CJS4	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0026	0.0026	-0.0006	-0.0005	0.7910	0.9008	0.9851	0.9993
UniRef90_R5CJS4|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0026	0.0026	-0.0006	-0.0005	0.7910	0.9008	0.9851	0.9993
UniRef90_F3BB74	Rumgna_00694	UniRef50_R5TQC2	0.0000	0.0000	0.0000	0.0000	0.0104	-0.0005	-0.0005	0.9321	0.9549	0.9851	0.9993
UniRef90_R6HKH7	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0104	0.0026	-0.0005	-0.0036	0.9073	0.5577	0.9851	0.9993
UniRef90_R6HKH7|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0104	0.0026	-0.0005	-0.0036	0.9073	0.5577	0.9851	0.9993
UniRef90_F3BB74|g__Lachnospiraceae_noname|s__Lachnospiraceae_bacterium_2_1_46FAA	Rumgna_00694	UniRef50_R5TQC2	0.0000	0.0000	0.0000	0.0000	0.0104	-0.0003	-0.0003	0.9334	0.9551	0.9851	0.9993
UniRef90_F3BB74|unclassified	Rumgna_00694	UniRef50_R5TQC2	0.0000	0.0000	0.0000	0.0000	0.0078	-0.0003	-0.0002	0.9079	0.9442	0.9851	0.9993
UniRef90_R5FS88	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0000	0.0026	-0.0001	0.0001	0.8254	0.9491	0.9851	0.9993
UniRef90_R5FS88|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0000	0.0026	-0.0001	0.0001	0.8254	0.9491	0.9851	0.9993
UniRef90_R7NI08	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0026	0.0000	-0.0001	-0.0007	0.9404	0.5326	0.9851	0.9993
UniRef90_R7NI08|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0026	0.0000	-0.0001	-0.0007	0.9404	0.5326	0.9851	0.9993
UniRef90_R7KB31	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0026	0.0000	0.0000	-0.0005	0.9784	0.6575	0.9851	0.9993
UniRef90_R7KB31|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0026	0.0000	0.0000	-0.0005	0.9784	0.6575	0.9851	0.9993
UniRef90_R5TQC2	Rumgna_00694	UniRef50_R5TQC2	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.0000	0.9851	0.9883	0.9851	0.9993
UniRef90_R5TQC2|unclassified	Rumgna_00694	UniRef50_R5TQC2	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.0000	0.9851	0.9883	0.9851	0.9993
UniRef90_R6D564	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0000	0.0052	0.0001	0.0000	0.9498	0.9958	0.9851	0.9993
UniRef90_R6D564|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0000	0.0052	0.0001	0.0000	0.9498	0.9958	0.9851	0.9993
UniRef90_C4FBF0|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0000	0.0000	0.0000	0.0052	0.0000	0.0002	-0.0019	0.8917	0.4528	0.9851	0.9993
UniRef90_R5TKT5|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0018	0.0000	0.0000	0.0000	0.0018	0.0000	0.0915	0.9910	0.2775	0.9993
UniRef90_R6UAF4|g__Clostridium|s__Clostridium_sp_HGF2	Rumgna_00694	UniRef50_R5TQC2	0.0056	0.0000	0.0000	0.0000	0.0000	0.0018	0.0000	0.0068	0.9883	0.0263	0.9993

Table S9 - Rumgna_genes_mgx (continued)

UniRef90_R6UAF4|g__Peptostreptococcaceae_noname|s__Clostridium_difficile	Rumgna_00694	UniRef50_R5TQC2	0.0056	0.0000	0.0000	0.0000	0.0000	0.0018	0.0000	0.0068	0.9883	0.0263	0.9993
UniRef90_R9N7L8	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0072	0.0000	0.0000	0.0026	0.0024	0.0002	0.5733	0.9724	0.9746	0.9993
UniRef90_R9N7L8|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0072	0.0000	0.0000	0.0026	0.0024	0.0002	0.5733	0.9724	0.9746	0.9993
UniRef90_R6ZBB2	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0018	0.0000	0.0026	0.0000	0.0028	-0.0052	0.4915	0.4090	0.9294	0.9993
UniRef90_R6ZBB2|g__Coriobacteriaceae_noname|s__Coriobacteriaceae_bacterium_phI	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0018	0.0000	0.0026	0.0000	0.0028	-0.0052	0.4915	0.4090	0.9294	0.9993
UniRef90_R5TKT5|g__Blautia|s__Ruminococcus_gnavus	Rumgna_02133	UniRef50_R5B9W8	0.4068	0.3009	0.3922	0.2254	0.1671	0.0032	0.0703	0.9634	0.4545	0.9851	0.9993
UniRef90_R9K3B3	Rumgna_02133	UniRef50_R5B9W8	0.0282	0.0180	0.0000	0.0181	0.0235	0.0048	-0.0164	0.6957	0.3935	0.9851	0.9993
UniRef90_R9K3B3|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0282	0.0180	0.0000	0.0181	0.0235	0.0048	-0.0164	0.6957	0.3935	0.9851	0.9993
UniRef90_B1CB64	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0000	0.0196	0.0000	0.0000	0.0068	0.0053	0.0105	0.2275	0.0377	0.8159
UniRef90_B1CB64|g__Anaerofustis|s__Anaerofustis_stercorihominis	Rumgna_02133	UniRef50_R5B9W8	0.0056	0.0000	0.0196	0.0000	0.0000	0.0068	0.0053	0.0105	0.2275	0.0377	0.8159
UniRef90_R5TKT5	Rumgna_02133	UniRef50_R5B9W8	0.4181	0.3045	0.3922	0.2383	0.1749	0.0083	0.0248	0.9094	0.8034	0.9851	0.9993
UniRef90_R6UAF4|g__Erysipelotrichaceae_noname|s__Erysipelotrichaceae_bacterium_3_1_53	Rumgna_00694	UniRef50_R5TQC2	0.0169	0.0072	0.0000	0.0000	0.0026	0.0092	-0.0003	0.1364	0.9737	0.3834	0.9993
UniRef90_U2C7T4	Rumgna_02133	UniRef50_R5B9W8	0.0621	0.1171	0.0980	0.0829	0.0313	0.0094	-0.0558	0.8397	0.3773	0.9851	0.9993
UniRef90_R6UAF4|unclassified	Rumgna_00694	UniRef50_R5TQC2	0.0169	0.0000	0.0000	0.0000	0.0000	0.0098	0.0001	0.0050	0.9838	0.0219	0.9993
UniRef90_R9MDG8	Rumgna_02133	UniRef50_R5B9W8	0.0452	0.0198	0.0000	0.0259	0.0261	0.0122	-0.0173	0.3997	0.4423	0.8313	0.9993
UniRef90_R9MDG8|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0452	0.0198	0.0000	0.0259	0.0261	0.0122	-0.0173	0.3997	0.4423	0.8313	0.9993
UniRef90_B9Y5C1|unclassified	Rumgna_00694	UniRef50_R5TQC2	0.0226	0.0000	0.0000	0.0000	0.0026	0.0124	-0.0001	0.0000	0.9828	0.0000	0.9993
UniRef90_R6UAF4|g__Erysipelotrichaceae_noname|s__Erysipelotrichaceae_bacterium_6_1_45	Rumgna_00694	UniRef50_R5TQC2	0.0678	0.0162	0.0980	0.0104	0.0183	0.0163	0.0734	0.3374	0.0020	0.7797	0.0700
UniRef90_R6UAF4|g__Erysipelotrichaceae_noname|s__Erysipelotrichaceae_bacterium_21_3	Rumgna_00694	UniRef50_R5TQC2	0.0621	0.0072	0.0784	0.0104	0.0052	0.0172	0.0441	0.2879	0.0550	0.6804	0.3367
UniRef90_R6R2D2	Rumgna_02133	UniRef50_R5B9W8	0.0621	0.0324	0.0980	0.0466	0.0627	0.0194	0.0113	0.4309	0.7628	0.8618	0.9993
UniRef90_R6R2D2|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0621	0.0324	0.0980	0.0466	0.0627	0.0194	0.0113	0.4309	0.7628	0.8618	0.9993
UniRef90_H7CU74	Rumgna_02133	UniRef50_R5B9W8	0.0282	0.0054	0.0196	0.0026	0.0000	0.0305	0.0209	0.0001	0.0903	0.0009	0.4267
UniRef90_H7CU74|g__Clostridium|s__Clostridium_perfringens	Rumgna_02133	UniRef50_R5B9W8	0.0282	0.0054	0.0196	0.0026	0.0000	0.0305	0.0209	0.0001	0.0903	0.0009	0.4267
UniRef90_U5F5L7	Rumgna_02133	UniRef50_R5B9W8	0.0904	0.0631	0.2157	0.0648	0.0653	0.0322	-0.0006	0.3763	0.9907	0.8313	0.9993
UniRef90_R6UAF4|g__Erysipelotrichaceae_noname|s__Clostridium_innocuum	Rumgna_00694	UniRef50_R5TQC2	0.0847	0.0072	0.0196	0.0130	0.0026	0.0336	0.0111	0.0250	0.5978	0.0866	0.9993
UniRef90_S2XY50|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0678	0.0126	0.0196	0.0026	0.0026	0.0427	0.0070	0.0000	0.6139	0.0001	0.9993
UniRef90_S2XY50|g__Lachnospiraceae_noname|s__Lachnospiraceae_bacterium_4_1_37FAA	Rumgna_02133	UniRef50_R5B9W8	0.0452	0.0018	0.0000	0.0026	0.0026	0.0516	-0.0009	0.0001	0.9651	0.0008	0.9993
UniRef90_R6UAF4|g__Erysipelotrichaceae_noname|s__Erysipelotrichaceae_bacterium_2_2_44A	Rumgna_00694	UniRef50_R5TQC2	0.0791	0.0108	0.0980	0.0207	0.0131	0.0562	0.0623	0.0031	0.0258	0.0152	0.2179
UniRef90_S2XY50|g__Lachnospiraceae_noname|s__Lachnospiraceae_bacterium_9_1_43BFAA	Rumgna_02133	UniRef50_R5B9W8	0.1130	0.0090	0.0000	0.0052	0.0026	0.0601	0.0003	0.0007	0.9911	0.0040	0.9993
UniRef90_U5F5L7|g__Erysipelotrichaceae_noname|s__Erysipelotrichaceae_bacterium_5_2_54FAA	Rumgna_02133	UniRef50_R5B9W8	0.0226	0.0090	0.1765	0.0233	0.0000	0.0604	0.0163	0.0001	0.4467	0.0009	0.9993
UniRef90_U2C7T4|unclassified	Rumgna_02133	UniRef50_R5B9W8	0.0565	0.0450	0.0196	0.0363	0.0261	0.0832	-0.0335	0.0006	0.3283	0.0036	0.9993
UniRef90_R6UAF4	Rumgna_00694	UniRef50_R5TQC2	0.1864	0.0324	0.0980	0.0311	0.0287	0.1394	0.0821	0.0000	0.0382	0.0000	0.2577
UniRef90_S2XY50	Rumgna_02133	UniRef50_R5B9W8	0.1977	0.0216	0.0196	0.0104	0.0052	0.1612	0.0108	0.0000	0.7652	0.0000	0.9993

Table S9 - BF3538_mgx

HUMAnN2 Homolog + Stratification	Query Gene ID	UniRef50	pre.CD-dys	pre.CD-nondys	pre.UC-dys	pre.UC-nondys	prev.nonIBD-nondys	coef.CD-dys	coef.UC-dys	pval.CD-dys	pval.UC-dys	qval.CD-dys	qval.UC-dys
UniRef90_E1WV34	BF3538	UniRef50_E1WV34	0.3107	0.4324	0.3137	0.3497	0.3185	-0.1870	-0.3871	0.0087	0.0000	0.0261	0.0001
UniRef90_E1WV34|g__Bacteroides|s__Bacteroides_fragilis	BF3538	UniRef50_E1WV34	0.3107	0.4324	0.3137	0.3446	0.3159	-0.1871	-0.3866	0.0084	0.0000	0.0261	0.0001
UniRef90_E1WV34|g__Bacteroides|s__Bacteroides_sp_3_2_5	BF3538	UniRef50_E1WV34	0.0056	0.0018	0.0000	0.0000	0.0235	0.0006	0.0000	0.9485	0.9993	0.9485	0.9993
UniRef90_E1WV34|unclassified	BF3538	UniRef50_E1WV34	0.0282	0.0090	0.0196	0.0155	0.0026	0.0140	0.0095	0.1781	0.5764	0.3562	0.6917
UniRef90_R5RWD9	BF3538	UniRef50_E1WV34	0.0452	0.0360	0.0784	0.0596	0.0000	0.0124	-0.0336	0.4799	0.1410	0.5758	0.2115
UniRef90_R5RWD9|g__Bacteroides|s__Bacteroides_fragilis	BF3538	UniRef50_E1WV34	0.0452	0.0360	0.0784	0.0596	0.0000	0.0124	-0.0336	0.4799	0.1410	0.5758	0.2115

Supplementary Table 10 | Differential abundance modeling of species with 3α-/3β-HSDH homologs in HMP2. Table fields follow the same format as Supplementary Information Table 9 (detailed above) without the 'class' field.

species	pre.CD-dys	pre.CD-nondys	pre.UC-dys	pre.UC-nondys	pre.nonIBD-nondys	coef.CD-dys	coef.UC-dys	pval.CD-dys	pval.UC-dys	qval.CD-dys	qval.UC-dys
Adlercreutzia_equolifaciens	0.04519774	0.066666667	0.039215686	0.10880829	0.161879896	-0.095280005	-0.018421386	0.115874981	0.826534144	0.202781217	0.826534144
Bacteroides_cellulosilyticus	0.06779661	0.358558559	0.176470588	0.341968912	0.441253264	-0.244964165	-0.28521006	0.003337869	0.008327685	0.008761907	0.031264721
Bacteroides_dorei	0.412429379	0.666666667	0.62745098	0.652849741	0.796344648	-0.741864941	-0.181390829	6.43E-11	0.215956759	4.50E-10	0.302339463
Bacteroides_fragilis	0.457627119	0.645045045	0.549019608	0.533678756	0.527415144	-0.61688588	-0.761459857	1.50E-05	4.29E-05	7.90E-05	0.000450683
Bacteroides_intestinalis	0.04519774	0.172972973	0	0.106217617	0.125326371	-0.04394252	-0.059681073	0.3909779	0.369828381	0.58646685	0.456846823
Bacteroides_uniformis	0.598870056	0.936936937	0.607843137	0.914507772	0.934725849	-1.199319275	-0.673457777	3.65E-26	4.10E-06	7.67E-25	8.61E-05
Bacteroides_vulgatus	0.740112994	0.924324324	0.843137255	0.948186528	0.966057441	-0.933533454	-0.249291185	2.46E-21	0.048381849	2.58E-20	0.107090565
Bifidobacterium_pseudocatenulatum	0.033898305	0.189189189	0.098039216	0.111398964	0.164490862	-0.125890139	-0.06113882	0.096339207	0.546183713	0.183920305	0.603676736
Catenibacterium_mitsuokai	0.011299435	0.068468468	0	0.010362694	0.057441253	-0.019473213	-0.012038734	0.287458109	0.609420567	0.464355408	0.639891596
Clostridium_bolteae	0.774011299	0.747747748	0.784313725	0.79015544	0.537859008	-0.238484829	-0.338418712	0.074784155	0.057753542	0.157046726	0.110256761
Clostridium_citroniae	0.192090395	0.340540541	0.137254902	0.313471503	0.25848564	-0.200713759	-0.323093724	0.039348582	0.015652418	0.091813358	0.046957253
Clostridium_innocuum	0.129943503	0.028828829	0.058823529	0.080310881	0.026109661	-0.004560498	-0.049939383	0.919363197	0.421096189	0.965331357	0.491278888
Clostridium_scindens	0.09039548	0.068468468	0.039215686	0.062176166	0.096605744	0.007855126	-0.10848664	0.863852421	0.083603735	0.954784255	0.146306536
Collinsella_aerofaciens	0.192090395	0.565765766	0.254901961	0.554404145	0.64229765	-0.386254564	-0.274874344	4.26E-05	0.026130731	0.000178956	0.068593168
Collinsella_intestinalis	0.04519774	0.043243243	0.117647059	0.090673575	0.028720627	-0.108742319	-0.125633981	0.003090799	0.008932778	0.008761907	0.031264721
Eggerthella_lenta	0.118644068	0.041441441	0	0.025906736	0.018276762	-0.011704783	-0.066596964	0.746871705	0.181417694	0.915616498	0.272126541
Gordonibacter_pamelaeae	0.005649718	0.009009009	0	0.023316062	0.020887728	-0.000713535	-0.029115134	0.968528731	0.288585251	0.968528731	0.378768142
Parabacteroides_merdae	0.214689266	0.630630631	0.215686275	0.668393782	0.618798956	-0.392522235	-0.350067731	8.23E-05	0.006654119	0.000287893	0.031264721
Peptoniphilus_harei	0	0.005405405	0	0.025906736	0.007832898	-0.004679827	-0.036509825	0.784814141	0.136508428	0.915616498	0.220513615
Pseudoflavonifractor_capillosus	0.129943503	0.147747748	0.117647059	0.18134715	0.279373368	0.029500081	-0.155222993	0.621468627	0.050995507	0.815677573	0.107090565
Ruminococcus_gnavus	0.768361582	0.607207207	0.882352941	0.603626943	0.467362924	0.098122606	0.458889809	0.433419916	0.005888036	0.606787882	0.031264721

Supplementary Table 11a - qPCR results for 16s rRNA gene to confirm successful colonization for the second set of experiment in Fig. 4b.

Sample #	*E.lenta*	Diet	Target	Ct values	Feces (mg)
1	DSM 2243	Control	E.lenta 16s	25.82	36.6
2	DSM 2243	Control	E.lenta 16s	24.86	81.6
3	DSM 2243	LCA	E.lenta 16s	24.96	80.0
4	DSM 2243	LCA	E.lenta 16s	23.62	120.3
5	DSM 2243	LCA	E.lenta 16s	22.99	60.5
6	DSM 15644	Control	E.lenta 16s	25.50	50.8
7	DSM 15644	Control	E.lenta 16s	26.21	65.9
8	DSM 15644	LCA	E.lenta 16s	27.06	51.7
9	DSM 15644	LCA	E.lenta 16s	25.35	89.7
10	DSM 15644	LCA	E.lenta 16s	26.17	92.8

Supplementary Table 11b - qPCR results for 16s rRNA gene to confirm successful colonization for the second sets of experiment in Fig. 4c.

Sample #	*E.lenta*	2nd bacteria	Target	Ct value	Target	Ct value	Feces (mg)
1	-	-	E.lenta 16s	-	B.fragilis 16s	-	25.9
2	-	-	E.lenta 16s	33.63	B.fragilis 16s	-	23.2
3	-	-	E.lenta 16s	32.87	B.fragilis 16s	-	39.0
4	-	-	E.lenta 16s	-	B.fragilis 16s	-	26.80
17	DSM 2243	*B.fragilis*	E.lenta 16s	22.52	B.fragilis 16s	15.13	35.20
18	DSM 2243	*B.fragilis*	E.lenta 16s	24.08	B.fragilis 16s	15.04	48.50
19	DSM 2243	*B.fragilis*	E.lenta 16s	23.86	B.fragilis 16s	15.65	33.20
20	DSM 2243	*B.fragilis*	E.lenta 16s	24.28	B.fragilis 16s	16.77	101.5
56	-	*B.fragilis*	E.lenta 16s	not determined	B.fragilis 16s	23.88	87
57	-	*B.fragilis*	E.lenta 16s	not determined	B.fragilis 16s	23.24	96
58	-	*B.fragilis*	E.lenta 16s	not determined	B.fragilis 16s	23.15	80

Supplementary table 12 | Deposition of standards in MoNA - MassBank of North America.

Compound	Compound_ID_Short	Chemical Formula	RT	MZ	RT_MS2	MZ_MS2	SMILES	MoNa_Deposition	Adduct	Neutral	[M+H]	[M+NH4]	[M+Na]	[M-H]	[M-H2O+H]
3-oxo lithocholic acid	3oxoLCA	C24H38O3	12.49	373.2748	12.49	373.2748	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@H]4[C@@]3(CCC(=O)C4)C)C	MoNA031840	[M-H]-	374.2821	375.2894	392.3159	397.2713	373.2748	357.2788
isolithocholic acid	isoLCA	C24H40O3	11.54	375.2905	11.54	375.2905	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@@H](C4)O)C)C	MoNA031841	[M-H]-	376.2977	377.305	394.3316	399.287	375.2905	359.294457
lithocholic acid	LCA	C24H40O3	12.24	375.2904	12.24	375.2904	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@H](C4)O)C)C	MoNA031842	[M-H]-	376.2977	377.305	394.3316	399.287	375.2905	359.294457
allolithocholic acid	alloLCA	C24H40O3	12.29	375.2904	12.29	375.2904	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@@H]4[C@@]3(CC[C@H](C4)O)C)C	MoNA031843	[M-H]-	376.2977	377.305	394.3316	399.287	375.2905	359.294457
isoallolithocholic acid	isoalloLCA	C24H40O3	11.42	375.2904	11.42	375.2904	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@@H]4[C@@]3(CC[C@@H](C4)O)C)C	MoNA031844	[M-H]-	376.2977	377.305	394.3316	399.287	375.2905	359.294457
3oxo deoxycholic acid	3oxoDCA	C24H38O4	10.44	389.2697	10.44	389.2697	C[C@H](CCC(=O)O)[C@@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CCC(=O)C4)C)O)O)C	MoNA031845	[M-H]-	390.277	391.2843	408.3108	413.2662	389.2697	373.2737215
iso deoxycholic acid	isoDCA	C24H40O4	9.38	391.2853	9.38	391.2853	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CCCC4)C)O)O)C	MoNA031846	[M-H]-	392.2927	393.2999	410.3265	415.2819	391.2854	375.2893716
deoxycholic acid	DCA	C24H40O4	10.44	391.2853	10.44	391.2853	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C	MoNA031847	[M-H]-	392.2927	393.2999	410.3265	415.2819	391.2854	375.2893716
3-oxo lithocholic acid	3oxoLCA	C24H38O3	12.49	357.2788	12.49	357.2788	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@H]4[C@@]3(CCC(=O)C4)C)C	MoNA031848	[M-H2O+H]+	374.2821	375.2894	392.3159	397.2713	373.2748	357.2788
isolithocholic acid	isoLCA	C24H40O3	11.54	359.294457	11.54	359.294457	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@@H](C4)O)C)C	MoNA031849	[M-H2O+H]+	376.2977	377.305	394.3316	399.287	375.2905	359.294457
lithocholic acid	LCA	C24H40O3	12.24	359.294457	12.24	359.294457	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@H](C4)O)C)C	MoNA031850	[M-H2O+H]+	376.2977	377.305	394.3316	399.287	375.2905	359.294457
allolithocholic acid	alloLCA	C24H40O3	12.29	359.294457	12.29	359.294457	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@@H]4[C@@]3(CC[C@H](C4)O)C)C	MoNA031855	[M-H2O+H]+	376.2977	377.305	394.3316	399.287	375.2905	359.294457
isoallolithocholic acid	isoalloLCA	C24H40O3	11.42	359.294457	11.42	359.294457	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC[C@@H]4[C@@]3(CC[C@@H](C4)O)C)C	MoNA031851	[M-H2O+H]+	376.2977	377.305	394.3316	399.287	375.2905	359.294457
3oxo deoxycholic acid	3oxoDCA	C24H38O4	10.44	373.2737215	10.44	373.2737215	C[C@H](CCC(=O)O)[C@@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CCC(=O)C4)C)O)O)C	MoNA031852	[M-H2O+H]+	390.277	391.2843	408.3108	413.2662	389.2697	373.2737215
iso deoxycholic acid	isoDCA	C24H40O4	9.38	375.2893716	9.38	375.2893716	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CCCC4)C)O)O)C	MoNA031853	[M-H2O+H]+	392.2927	393.2999	410.3265	415.2819	391.2854	375.2893716
deoxycholic acid	DCA	C24H40O4	10.44	375.2893716	10.44	375.2893716	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C	MoNA031854	[M-H2O+H]+	392.2927	393.2999	410.3265	415.2819	391.2854	375.2893716

References

56 Varasi, M.; Walker, K. A. M.; Maddox, M. L. A Revised Mechanism for the Mitsunobu Reaction. J. Org. Chem. 52, 4235–4238, doi:10.1021/jo00228a016 (1987).

57 Yang, J.; Cheng, Y.; Shi, Z.; Zhao, Z. Synthesis of Novel Triazole Derivatives of Methyl 3-Oxocholanate Using Microwave Irradiation. *Journal of Chemical Research* **34**, 680–683, doi:10.3184/030823410X12857507693328 (2010).

58 Fujioka, H.; Okitsu, T.; Ohnaka, T.; Sawama, Y.; Kubo, O.; Okamoto, K.; Kita, Y. Reaction of Tetrahydropyranyl Ethers with Triethylsilyl Trifluoromethanesulfonate–2,4,6-Collidine Combination: Speculation on the Intermediate, Efficient Deprotection, and Application to Efficient Ring-Closing Metathesis as a Tether. *Adv. Synth. Catal.* **349**, 636–646, doi:10.1002/adsc.200600572 (2007).

59 Miro, P.; Vayá, I.; Sastre, G.; Jiménez, M. C.; Marin, M. L.; Miranda, M. A. Triplet Energy Management Between Two Signaling Units Through Cooperative Rigid Scaffolds. *Chem. Commun.* **52**, 713–716, doi:10.1039/C5CC08102E (2016).

60 Bisanz, J. E. et al. A Genomic Toolkit for the Mechanistic Dissection of Intractable Human Gut Bacteria. Cell Host Microbe 27, 1001-1013.e9 (2020).

61 Lloyd-Price, J. et al. Multi-omics of the gut microbial ecosystem in inflammatory bowel diseases. Nature 569, 655–662 (2019).

62 Revu, S. et al. IL-23 and IL-1β Drive Human Th17 Cell Differentiation and Metabolic Reprogramming in Absence of CD28 Costimulation. Cell Reports 22, 2642–2653 (2018).