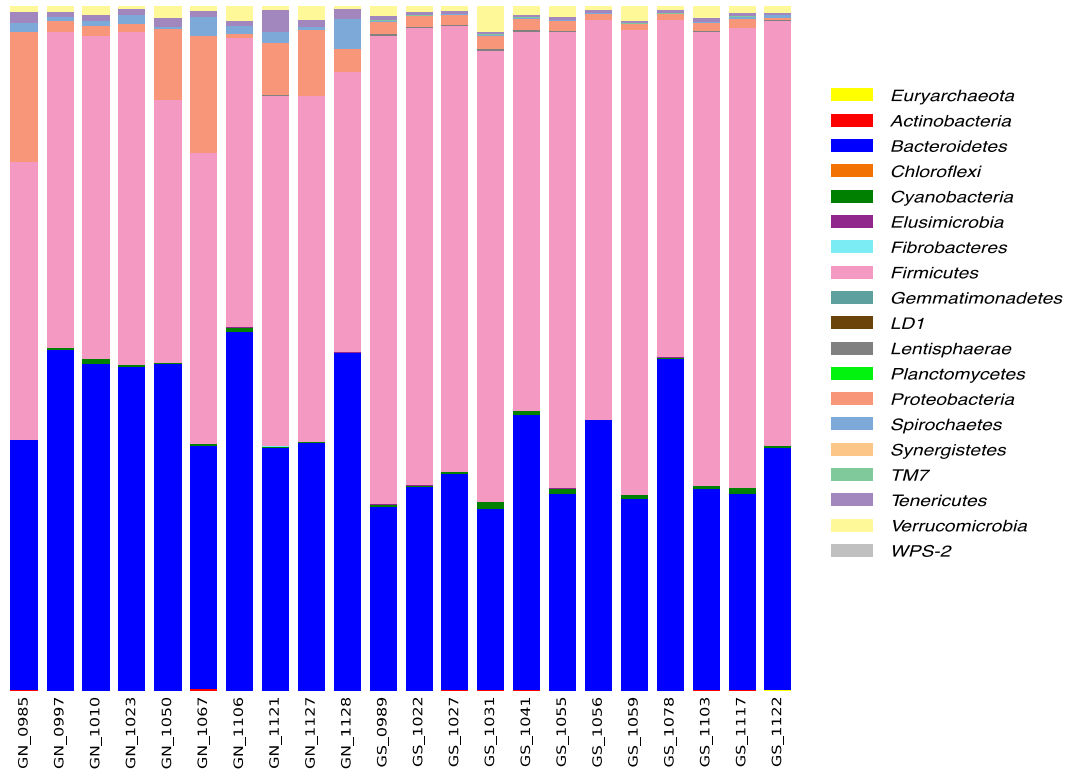


**Additional file 1**

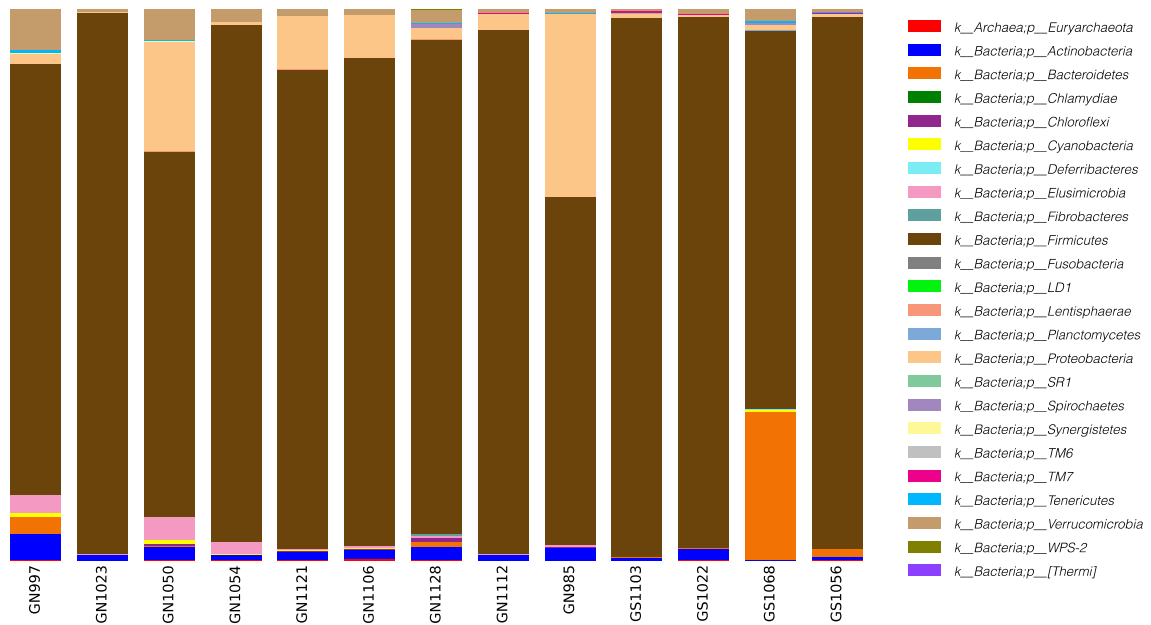


**Figure S1** Phylum-level fecal microbial composition in young beef cattle. The first ten samples were grain-fed (GN) individual cattle; the last 12 individuals were grass-fed (GS) cattle.

**Table S1** Selected 20 significantly different OTUs in relative abundance in the fecal microbiome of grain-fed and grass-fed Angus beef cattle. The OTU was identified based on Greengenes 16S rRNA database version 13\_8. The numbers denoted the relative abundance (Mean  $\pm$  SD) of corresponding OTUs in the grain-fed and grass-fed group. The LDA log<sub>10</sub> score was the calculated logarithm of LDA scores using the LefSe algorithm.

GreenGenes ID	Grain-fed	Grass-fed	LDA log <sub>10</sub> score	Annotation (Domain Phylum Class Order Family Genus Species)
327184	0.0077 $\pm$ 0.0043	0.0319 $\pm$ 0.0069	4.08	Bacteria Firmicutes Clostridia Clostridiales
509709	0.0078 $\pm$ 0.0039	0.0289 $\pm$ 0.0069	4.03	Bacteria Firmicutes Clostridia Clostridiales Lachnospiraceae
199226	0.0103 $\pm$ 0.0066	0.0213 $\pm$ 0.0092	3.78	Bacteria Firmicutes Clostridia Clostridiales Ruminococcaceae
298717	0.0178 $\pm$ 0.0123	0.0115 $\pm$ 0.0055	3.44	Bacteria Firmicutes Clostridia Clostridiales Ruminococcaceae
330414	0.0253 $\pm$ 0.0340	0.0000 $\pm$ 0.0000	4.08	Bacteria Firmicutes Clostridia Clostridiales
1112614	0.0203 $\pm$ 0.0208	0.0038 $\pm$ 0.0008	3.92	Bacteria Firmicutes Clostridia Clostridiales Ruminococcaceae
85199	0.0172 $\pm$ 0.0098	0.0060 $\pm$ 0.0020	3.74	Bacteria Firmicutes Clostridia Clostridiales Veillonellaceae
146314	0.0233 $\pm$ 0.0409	0.0000 $\pm$ 0.0000	4.05	Bacteria Tenericutes Mollicutes RF39
341737	0.0125 $\pm$ 0.0048	0.0075 $\pm$ 0.0026	3.33	Bacteria Firmicutes Clostridia Clostridiales

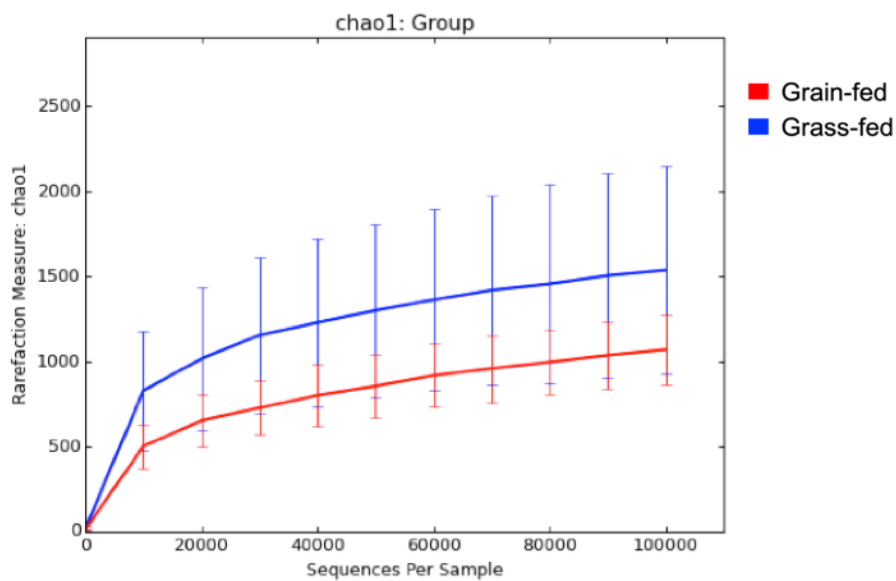
177109	0.0069 ± 0.0041	0.0110 ± 0.0031	3.28	Bacteria Firmicutes Clostridia Clostridiales Ruminococcaceae Oscillospira
593357	0.0062 ± 0.0019	0.0114 ± 0.0060	3.38	Bacteria Bacteroidetes Bacteroidia Bacteroidales Prevotellaceae Prevotella
323737	0.0111 ± 0.0061	0.0044 ± 0.0014	3.53	Bacteria Firmicutes Clostridia Clostridiales Ruminococcaceae
248126	0.0160 ± 0.0144	0.0000 ± 0.0000	3.90	Bacteria Firmicutes Clostridia Clostridiales Peptostreptococcaceae
554560	0.0115 ± 0.0061	0.0036 ± 0.0014	3.60	Bacteria Firmicutes Clostridia Clostridiales Ruminococcaceae
287909	0.0004 ± 0.0010	0.0127 ± 0.0076	3.79	Bacteria Firmicutes Clostridia Clostridiales
287798	0.0083 ± 0.0032	0.0056 ± 0.0016	3.12	Bacteria Firmicutes Erysipelotrichi Erysipelotrichales Erysipelotrichaceae
341730	0.0091 ± 0.0037	0.0049 ± 0.0015	3.32	Bacteria Firmicutes Clostridia Clostridiales Lachnospiraceae Coprococcus
332778	0.0036 ± 0.0014	0.0093 ± 0.0022	3.45	Bacteria Firmicutes Clostridia Clostridiales Lachnospiraceae
2051	0.0125 ± 0.0098	0.0016 ± 0.0016	3.76	Bacteria Bacteroidetes Bacteroidia Bacteroidales Prevotellaceae Prevotella
353691	0.0073 ± 0.0031	0.0057 ± 0.0007	2.80	Bacteria Firmicutes Erysipelotrichi Erysipelotrichales Erysipelotrichaceae



**Figure S2** Phylum-level microbial composition of jejunal digesta. The first nine samples were grain-fed (GN) individual cattle, and the last four individuals were cattle from grass-fed (GS) group.

**Table S2** Alpha diversity indices of jejunum microbiota in grass-fed and grain-fed Angus beef cattle. Welch's t-tests were used to calculate p-values.

Diversity Indices	Grain-fed	Grass-fed	p-value
Chao1	1225.62 ± 468.55	1536.97 ± 706.42	0.4575
Shannon	4.07 ± 0.95	4.69 ± 2.40	0.6468
Simpson	0.83 ± 0.08	0.990 ± 0.11	0.9238
PD_whole_tree	49.02 ± 9.46	66.77 ± 18.04	0.1416



**Figure S3** Rarefaction curves of jejunal microbiome based on Chao1 values of grass-fed (blue) and grain-fed (red) groups.

**Table S3** Eleven bile acids identified from bile in the gallbladder of grass-fed and grain-fed cattle that did not show significant differences ( $p > 0.05$ ). The concentration Unit showed as  $\mu\text{mol/ml}$ .

<b>Bile acids</b>	<b>Grain-fed</b>	<b>Grass-fed</b>	<b>p-value</b>
7-Ketodeoxycholic acid	$0.08 \pm 0.057$	$0.382 \pm 0.425$	0.0699
Deoxycholic acid	$0.828 \pm 0.056$	$0.774 \pm 0.076$	0.1612
Ursodeoxycholic acid	$0.211 \pm 0.028$	$0.201 \pm 0.012$	0.2352
Glycohyodeoxycholic acid	$0.021 \pm 0.009$	$0.018 \pm 0.005$	0.2574
Glycochenodeoxycholic acidt	$19.651 \pm 12.122$	$16.631 \pm 3.081$	0.3142
Taurochenodexycholic acid	$15.947 \pm 7.29$	$14.868 \pm 2.207$	0.4117
$\alpha$ -Muricholic acid	$0.062 \pm 0.029$	$0.078 \pm 0.033$	0.461
Tauro-III-muricholic acid	$0.164 \pm 0.145$	$0.143 \pm 0.061$	0.5654
Tauro- $\alpha$ -muricholic acid	$0.018 \pm 0.009$	$0.017 \pm 0.008$	0.6432
Apocholic acid	$0.043 \pm 0.028$	$0.038 \pm 0.043$	0.7804
Dehydrolithocholic acid	$0.032 \pm 0.008$	$0.036 \pm 0.007$	0.783
III-muricholic acid	$0.07 \pm 0.009$	$0.073 \pm 0.018$	0.7948

**Figure S4** Demonstration of global balances for secondary bile acids quantities of grass-fed and grain-fed cattle. The regression model was analyzed for each type of secondary bile acids. Microbiome signatures, including taxa in both denominator and numerator, were specified at the top of each figure. (A) Glycodeoxycholic\_acid. (B) Glycolithocholic\_acid. (C) Glycoursodeoxycholic\_acid. (D) Taurodeoxycholic\_acid. (E) Tauroolithocholic\_acid. (F) Total of tauroursodeoxycholic/taurohyodeoxycholic acid.

