

Supplemental Material, Table S1. ^1H NMR chemical shifts for metabolites assigned in liver, fecal and cecal content extracts

key	metabolites	moieties	δ ^1H (ppm) and multiplicity ^a	Samples ^b
1	Lipid	CH_3 , $(\text{CH}_2)_n$, $\text{CH}_2\text{-C}=\text{C}$, $\text{CH}_2\text{-C}=\text{O}$, $\text{C-CH}_2\text{-C=}$, -CH=CH-	0.89(m), 1.27(m), 2.0(m), 2.3(m), 2.78(m), 5.3(m)	L
2	Isoleucine	αCH , βCH , γCH_3 , δCH_3	3.65(d), 1.95(m), 0.99(t), 1.02(d)	L, F, C
3	Leucine	αCH , βCH_2 , γCH_3 , δCH_3	0.94(d), 3.72(t), 1.96(m), 0.91(d)	L, F, C
4	Valine	αCH , βCH , γCH_3	3.6(d), 2.26(m), 0.98(d), 1.04(d)	L, F, C
5	D-3-hydroxybutyrate	CH , CH_2 , γCH_3 , CH_2	4.16(dt), 2.41(dd), 1.20(d), 2.31(dd)	L
6	Lactate	αCH , βCH_3	4.11(q), 1.32(d)	L, F, C
7	Alanine	αCH , βCH_3	3.77(q), 1.48(d)	L, F, C
8	Acetate	CH_3	1.91(s)	L, F, C
9	n-butyrate	CH_3 , CH_2 , CH_2	0.91(t), 1.56(m), 2.16(t)	F, C
10	Propionate	CH_3 , CH_2	1.06(t), 2.18(q)	F, C
11	Threonine	γCH_3 , αCH , βCH	1.33(d), 3.59(d), 4.26(m)	F, C
12	Glutamate	αCH , βCH_2 , γCH_2	2.08(m), 2.34(m), 3.75(m)	L
13	Glutamine	αCH , βCH_2 , γCH_2	2.15(m), 2.44(m), 3.77(m)	L, F
14	Glutathione	CH_2 , CH_2 , S-CH_2 , N-CH , CH	2.16(m), 2.55(m), 2.95(dd), 3.78(m), 4.56(q)	L

15	L-arginine	γCH_2 , βCH_2 , αCH	1.72(m), 1.93(m), 3.77(m)	F
16	L-proline	CH_2 , CH_2 , CH	2.05(m), 2.34(m), 3.4(m)	F, C
17	Creatine	CH_3 , CH_2	3.03(s), 3.93(s)	F, C
18	Choline	$\text{N}(\text{CH}_3)_3$, OCH_2 , NCH_2	3.2(s), 4.05(t), 3.51(t)	L, F, C
19	Phosphocholine (PC)	$\text{N}(\text{CH}_3)_3$, OCH_2 , NCH_2	3.22(s), 4.21(t), 3.61(t)	L
20	Glycerophosphocholine	$\text{N}(\text{CH}_3)_3$, OCH_2 , NCH_2	3.22(s), 4.32(t), 3.68(t)	L
21	β -Glucose	1-CH	4.66(d)	L
22	α -Glucose	1-CH	5.23(d)	L, F, C
23	Unsaturated fatty acid	$\text{CH}=\text{CH}$	2.73, 5.3	L
24	TMAO	CH_3	3.27(s)	L
25	Tyrosine	CH , CH	6.89(dd), 7.18(dd)	L, F, C
26	Histidine	2-CH, 4-CH, CH_2	7.75(t), 7.08(d), 6.05(d)	L, F, C
27	Phenylalanine	Ring-CH	7.40(m), 7.33(m), 7.35(m)	L, F, C
28	Formate	CH	8.45(s)	L, F, C
29	Betaine	CH_2 , CH_3	3.27(s), 3.93(s)	L
30	Glycogen	1-CH	5.38-5.45(m)	L
31	Bile acid	CH_3	0.73(m)	L, F, C
32	Lysine	αCH , βCH_2 , γCH_2 , δCH_2	3.76(t), 1.89(m), 1.72(m), 3.01(t)	L, F, C
33	N-acetyl aspartate	CH_3	2.01(s)	L
34	Oligosaccharides	αCH resonances	3.3-3.9	F, C

35	Succinate	CH ₃	2.41(s)	L, F, C
36	Taurine	S-CH ₂ , N-CH ₂	3.26(t), 3.40(t)	L, F, C
37	Glycine	CH ₂	3.57(s)	L, F, C
38	Inosine	14-CH, 1-CH, 8-CH, 4'-CH, 5'-CH, CH ₂ (1/2), CH ₂ (1/2)	8.34(s), 6.09(d), 8.22(s), 4.76(t), 4.47(m)	L
39	Uridine	11-CH, 7-CH, 12-CH, 6-CH, 5- CH, 4-CH, CH ₂ , CH ₂	7.88(d), 5.92(d), 5.9(d), 4.36(m), 4.24(t)	L, F, C
40	Fumarate	CH	6.53(s)	L, F, C
41	Nicotinurate	2-CH, 6-CH, 4-CH, 5-CH	8.93(s), 8.62(d), 8.25(d), 7.60(dd),	L, F, C
42	Adenosine	14-CH	8.32(s)	L, C
43	Uracil	1-CH, 2-CH	5.81(d), 7.54(d)	L, F, C
44	α-galactose	1-CH, 2-CH, 3-CH	5.28(d), 3.81(dd); 3.97(m)	F
45	α-arabinose	1-CH, 2-CH	5.21(d), 3.87(dd)	F
46	α-xylose	1-CH, 2-CH, 3-CH	5.20(d), 3.53(dd), 3.68(m)	F
47	Hypoxanthine	1-CH, 2-CH	8.20(s), 8.21(s)	F, C
48	Glucose & amino acids	αCH resonances	3.3-3.9	L
49	Ethanol	CH ₃ , CH ₂	1.18(t), 3.65(q)	C
50	Pyruvate	CH ₃	2.38(s)	F, C
51	TMA	CH ₃	2.88(s)	F, C
52	Raffinose	1-CH	5.41(d)	F, C
53	Stachyose	1-CH	5.41(d)	F, C

54	Methanol	CH ₃	3.36 (s)	F, C
55	Methionine	δCH ₃ , βCH ₂ , γCH ₂	2.14(s), 2.16(m), 2.65(t)	F, C
56	Urocanate	CHCOOH, CH(ring), 5CH	6.40(d), 7.31(d), 7.43(s)	F, C
57	Adenine	2CH, 6CH	8.19(s), 8.21(s)	F, C
58	α-ketoglutarate	γCH ₂ , βCH ₂	2.45(t), 3.01(t)	F, C

^a Key: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublet.

^b Liver (L), fecal (F) and cecal content (C) aqueous extracts.

Supplemental Material, Table S2. Significantly changed metabolites in the feces, cecal content, liver, and intestine of mice exposed to TCDF

Metabolite	Feces	Cecal content	Liver	Duodenum	Jejunum	Ileum	Cecum
	R ² X=0.64	R ² X=0.48	R ² X=0.74	R ² X=0.59	R ² X=0.48	R ² X=0.66	R ² X=0.56

	Q ² =0.88	Q ² =0.64	Q ² =0.75	Q ² =0.85	Q ² =0.65	Q ² =0.87	Q ² =0.73
Lipid	—	—	+0.78 ^a	+0.84	—	+0.78	—
UFA	—	—	+0.81	—	—	—	—
PUFA	—	—	+0.74	—	—	—	—
Alanine	+0.82	—	-0.83	—	+0.72	—	—
Isoleucine	+0.93	—	—	+0.81	+0.69	+0.86	+0.71
Leucine	+0.88	—	—	+0.78	+0.64	+0.83	+0.68
Valine	+0.79	—	—	+0.76	+0.64	+0.85	+0.67
Tyrosine	+0.94	+0.74	-0.73	+0.74	+0.77	+0.81	—
Phenylalanine	+0.92	+0.78	-0.72	+0.83	+0.79	+0.82	+0.84
Lysine	+0.85	—	—	+0.84	+0.71	+0.79	—
Glutamine	+0.71	—	—	—	—	—	+0.73
Glycine	—	—	-0.63	—	—	-0.72	-0.86
Glucose	-0.76	-0.79	-0.75	—	—	—	-0.63
Glycogen	—	—	+0.77	—	—	—	—
Lactate	—	—	-0.75	-0.77	-0.81	—	—
Succinate	+0.79	—	—	—	+0.84	—	—
Fumarate	—	—	—	-0.68	—	—	—

Creatine	—	—	—	—	—	-0.82	—
n-butyrate	+0.82	+0.92	—	—	—	—	—
Propionate	+0.68	+0.88	—	—	—	—	—
Taurine	—	—	—	-0.85	—	-0.84	—
Choline	-0.75	—	-0.80	—	—	-0.81	-0.82
PC/GPC	—	-0.76	-0.68	—	—	-0.85	-0.83
Inosine	—	—	-0.84	—	—	—	—
Hypoxanthine	—	—	-0.67	—	-0.65	-0.85	—
Uracil	—	—	—	—	—	-0.73	—
Uridine	—	—	—	—	-0.63	-0.66	—
Nicotinurate	—	—	-0.69	—	-0.67	-0.68	—
Allantoate	—	—	—	—	—	+0.78	—
Oligosaccharides	-0.81	-0.71	—	—	—	—	—

^a Correlation coefficient values obtained from OPLS-DA of treatment groups;

+ and – indicate a significant increase and decrease of metabolite levels in the treatment groups compared to the control mice; — no change.