**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 multiplicitya | Samplesb |
| 1 | Lipid | CH3, (CH2)n, CH2-C=C, CH2-C=O,C-CH2-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, γCH3, δCH3 | 3.65(d), 1.95(m), 0.99(t), 1.02(d) | L, F, C |
| 3 | Leucine | αCH, βCH2, γCH3, δCH3 | 0.94(d), 3.72(t), 1.96(m), 0.91(d) | L, F, C |
| 4 | Valine | αCH, βCH, γCH3 | 3.6(d), 2.26(m), 0.98(d), 1.04(d) | L, F, C |
| 5 | D-3-hydroxybutyrate | CH, CH2, γCH3, CH2 | 4.16(dt),2.41(dd),1.20(d),2.31(dd) | L |
| 6 | Lactate | αCH, βCH3 | 4.11(q), 1.32(d) | L, F, C |
| 7 | Alanine | αCH, βCH3 | 3.77(q), 1.48(d) | L, F, C |
| 8  9  10  11 | Acetate  n-butyrate  Propionate  Threonine | CH3  CH3, CH2, CH2  CH3, CH2  γCH3, αCH, βCH | 1.91(s)  0.91(t), 1.56(m), 2.16(t)  1.06(t), 2.18(q)  1.33(d), 3.59(d), 4.26(m) | L, F, C  F, C  F, C  F, C |
| 12 | Glutamate | αCH, βCH2, γCH2 | 2.08(m), 2.34(m), 3.75(m) | L |
| 13 | Glutamine | αCH, βCH2, γCH2 | 2.15(m), 2.44(m), 3.77(m) | L, F |
| 14 | Glutathione | CH2, CH2, S-CH2, N-CH, CH | 2.16(m), 2.55(m), 2.95(dd), 3.78(m), 4.56(q) | L |
| 15  16  17 | L-arginine  L-proline  Creatine | γCH2, βCH2, αCH  CH2, CH2, CH  CH3, CH2 | 1.72(m), 1.93(m), 3.77(m)  2.05(m), 2.34(m), 3.4(m)  3.03(s), 3.93(s) | F  F, C  F, C |
| 18 | Choline | N(CH3)3, OCH2, NCH2 | 3.2(s), 4.05(t), 3.51(t) | L, F, C |
| 19 | Phosphocholine (PC) | N(CH3)3, OCH2, NCH2 | 3.22(s), 4.21(t), 3.61(t) | L |
| 20 | Glycerophosphocholine | N(CH3)3, OCH2, NCH2 | 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 | CH=CH | 2.73, 5.3 | L |
| 24 | TMAO | CH3 | 3.27(s) | L |
| 25 | Tyrosine | CH, CH | 6.89(dd), 7.18(dd) | L, F, C |
| 26 | Histidine | 2-CH, 4-CH, CH2 | 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 | CH2, CH3 | 3.27(s), 3.93(s) | L |
| 30 | Glycogen | 1-CH | 5.38-5.45(m) | L |
| 31 | Bile acid | CH3 | 0.73(m) | L, F, C |
| 32 | Lysine | αCH, βCH2, γCH2, δCH2 | 3.76(t), 1.89(m), 1.72(m), 3.01(t) | L, F, C |
| 33 | N-acetyl aspartate | CH3 | 2.01(s) | L |
| 34 | Oligosaccharides | αCH resonances | 3.3-3.9 | F, C |
| 35 | Succinate | CH3 | 2.41(s) | L, F, C |
| 36 | Taurine | S-CH2, N-CH2 | 3.26(t), 3.40(t) | L, F, C |
| 37 | Glycine | CH2 | 3.57(s) | L, F, C |
| 38 | Inosine | 14-CH, 1-CH, 8-CH, 4’-CH,  5’-CH, CH2(1/2), CH2(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, CH2, CH2 | 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  44  45  46 | Uracil  α-galactose  α-arabinose  α-xylose | 1-CH, 2-CH  1-CH, 2-CH, 3-CH  1-CH, 2-CH  1-CH, 2-CH, 3-CH | 5.81(d), 7.54(d)  5.28(d), 3.81(dd); 3.97(m)  5.21(d), 3.87(dd)  5.20(d), 3.53(dd), 3.68(m) | L, F, C  F  F  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 | CH3, CH2 | 1.18(t), 3.65(q) | C |
| 50 | Pyruvate | CH3 | 2.38(s) | F, C |
| 51 | TMA | CH3 | 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 | CH3 | 3.36 (s) | F, C |
| 55 | Methionine | δCH3, βCH2, γCH2 | 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 | γCH2, βCH2 | 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  R2X=0.64  Q2=0.88 | Cecal content  R2X=0.48  Q2=0.64 | Liver  R2X=0.74  Q2=0.75 | Duodenum  R2X=0.59  Q2=0.85 | Jejunum  R2X=0.48  Q2=0.65 | Ileum  R2X=0.66  Q2=0.87 | Cecum  R2X=0.56  Q2=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.