Molecule	^{1}H δ (ppm)	Moiety	Multiplicity
1. Bile salt 01	0.68	CH_3	s
2. Bile salt 02	0.70	CH_3	s
3. Bile salts 03	0.73	CH_3 (resonances partially overlapped)	s
4. U01	0.79		d
	0.94		
	1.28		
	1.77		
5. 2-Hydroxy-3-methylbutyrate	0.83	CH_3	d
	0.97	CH_3'	d
	2.01	Beta-CH	m
6. Butyrate	0.88	Gamma-CH_3	t
	1.56	Beta-CH_2	m
	2.16	Alpha-CH_2	t
7. Leu	0.97	CH_3, CH_3'	pt
	1.70	Beta-CH_2, gamma-CH	m
8. Val	0.99	CH_3	d
	1.04	CH_3'	d
	2.26	Beta-CH	m
	3.60	Alpha-CH	d
9. Ile	0.95	CH_3	t
	1.01	CH_3'	d
	1.26	Gamma-CH	m
	1.48	Gamma-CH'	m
	1.96	Beta-CH	m
10. Propionate	1.05	Beta-CH_3	t
	2.17	Alpha-CH_2	q
11. 2-Oxoisovalerate	1.13	CH_3, CH_3'	d
12. Ethanol	1.18	CH_3	t
	3.65	CH_2	q
13. U02	1.25	CH_3, CH_3'	d
	3.81		m
14. 3-Hydroxy-3-methylbutyrate (3-H	1.26	CH_3, CH_3'	s
15. Threonine (Thr)	1.33	Gamma-CH_3	d
	3.58	Alpha-CH	d
	4.25	Beta-CH	m
16. Acetoin	1.36	CH_3	d
17. 2-Aminoisobutyrate	1.48	CH_3, CH_3'	s
18. Alanine (Ala)	1.48	Beta-CH_3	d
	3.77	Alpha-CH	q
19. U03	1.65	Beta-CH_2	m
	2.24	Alpha-CH_2	t
	3.03	Gamma-CH_2	t
20. Acetate	1.92	CH_3	s
21. Glutamate (Glu)	2.04	Beta-CH	m
	2.11	Beta-CH'	m
	2.35	Gamma-CH_2	pt

22. Succinate	2.41	CH_2, CH_2'	s
23. 2-Ketoglutarate	2.44	Beta-CH_2	t
	3.02	Alpha-CH_2	t
24. U04	2.48	Alpha-CH_2	t
	2.85	Beta-CH_2	t
25. Trimethylamine (TMA)	2.91	CH_3, CH_3', CH_3''	s
26. Malonate	3.12	CH_2	s
27. Choline	3.20	CH_3, CH_3', CH_3''	bs
28. Taurine (Tau)	3.26	S-CH_2	t
	3.43	N-CH_2	t
29. U05	3.33	CH	t
	3.43		m
	3.62		m
	3.92		q
30. Methanol	3.36	CH_3	s
31. Glycine (Gly)	3.56	CH_2	s
32. Alpha-Glucose	3.52		m
	3.66		m
	5.19	1-CH	d
33. Alpha-Galactose	3.40		
	3.53		
	3.70		
	3.83		
	5.24	1-CH	d
34. Raffinose	5.42	1-CH Glucose	d
35. Uracil	5.80	CH	d
	7.55	CH	d
36. Fumarate	6.51	CH, CH'	s
37. 3-Hydroxyphenylacetate (3-HPA)	6.75	4-CH	dd
	6.80	2-CH	pt
	6.87	6-CH	m
	7.24	5-CH	t
38. 4-Hydroxyphenylacetate (4-HPA)	6.85	2-CH, 6-CH	pd
	7.17	3-CH, 5-CH	pd
39. Tyrosine (Tyr)	6.90	2-CH, 6-CH	d
	7.20	3-CH, 5-CH	d
40. Phenylalanine (Phe)	7.33-7.43	1-5 CH	m
41. Hypoxanthine	8.19	CH	s
	8.21	CH	s
42. Formate	8.46	CH	s
43. Nicotinate	7.52	CH	t
	8.25	CH	d
	8.61	CH	d
	8.94	CH	bs

Keynotes:

- Not quantifiable

- Integrated moiety

s: singlet; d: doublet; pd: pseudo-doublet; t: triplet; bs: broad singlet, m: multiplet; dd: doublet of doublets; pt: pseudo-triplet; q: quartet.

* Level 1: identified metabolites; level 2: putatively annotated compounds; level 3: putatively characterized compound classes; level 4: unknown compounds. The level of assignment has been reported according to Salek M. R. et al. doi: 10.1186/2047-217X-2-13

Supplementary Data 2: ^{1}H NMR assignment of mice's fecal

Level of Assignment*
3
3
3
1
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2
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3
2
3
3
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4
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waters.