Date of Issue:
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Reference Material 8048

Human Fecal Material

REFERENCE MATERIAL INFORMATION SHEET

Purpose: The non-certified values delivered by this Reference Material (RM) are intended for validating methods for routine metagenomic and metabolomic measurements, differential studies, interlaboratory comparisons, laboratory and instrument qualification, and training by the metagenomic and metabolomic communities. RM 8048 can be used to assess comparability within a laboratory, between laboratories, or among different measurement approaches. RM 8048 can also help assess the confidence of metagenomic and metabolite annotation and identification. NOTE: See page 26 for "Usage and Privacy Agreement" regarding identifiable private information.

Description: A unit of RM 8048 consists of four vials each from two dietary pools: Part A: Omnivore stool and Part B: Vegetarian stool. Each vial contains approximately 1 mL of stool slurry material (100 mg/mL cryohomogenized stool/water).

Non-Certified Values: Non-certified values are suitable for use in method development, method harmonization, and process control but do not provide metrological traceability to the International System of Units (SI) or other higher-order reference system [1].

Table 1 lists the moisture content of the omnivore and vegetarian stool. The moisture content was determined by freeze-drying 5 vials of each material continuously over a period of three days.

Non-certified metagenomic and metabolite identities (MSI level 2 [2]) present in RM 8048 are listed in Tables 2–7. These tables are also available as a download from the NIST store page, https://shop.nist.gov/ccrz__ProductDetails?sku=8048&cclcl=en_US. This information is the best metagenomic and metabolite annotation/identification estimate based on currently available information as determined by 16S rRNA amplicon sequencing, LC-MS/MS, and NMR; however, the evidence does not meet the NIST criteria for certification of chemical identity. Tables 2–3 list the identities of the metagenomic constituents in the omnivore and vegetarian stool that have been established using identification methodology generally accepted by experts in the field. The identified genus in RM 8048 is inferred from metagenomic analysis by DNA extraction and 16S rRNA amplicon sequencing. Tables 4–5 list the identities of metabolites in the omnivore and vegetarian stool that have been established using identification methodology generally accepted by experts in the field. The identified metabolites in RM 8048 are inferred from untargeted metabolomics analysis (liquid chromatography mass spectrometry data dependent acquisition). Samples were analyzed on two different high resolution mass spectrometer instruments and the resulting tandem MS spectra (MS/MS) were searched with three different mass spectral library search algorithms. Tables 6–7 list the identities of metabolites in the omnivore and vegetarian stool that have been established using identification methodology generally accepted by experts in the field. The identified metabolites in RM 8048 are inferred from two independent methods by NMR using a 600 MHz, 700 MHz and 900 MHz instrument respectively.

Additional Information: Additional information is provided in Appendix A.

Period of Validity: The non-certified values are valid within the measurement uncertainty specified until **31 January 2030.** The value assignments are nullified if the material is stored or used improperly, damaged, contaminated, or otherwise modified.

Maintenance of Non-Certified Values: NIST will monitor this material to the end of its period of validity. If substantive technical changes occur that affect the non-certified values during this period, NIST will update this Reference Material Information Sheet and notify registered users. RM users can register online from a link available on the NIST SRM website or fill out the user registration form that is supplied with the RM. Registration will facilitate notification. Before making use of any of the values delivered by this material, users should verify they have the most recent version of this documentation, available through the NIST SRM website (https://www.nist.gov/srm).

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Table 1. Non-Certified Moisture Content in Omnivore and Vegetarian Stool.

	Mass Fraction (%)
Moisture (Omnivore)	97.329 ± 0.426
Moisture (Vegetarian)	97.397 ± 0.420

Table 2. Non-Certified Top 50 V4 16S rRNA sequences and Genus-Species Identifications (listed alphabetically by genus) in Omnivore Stool

No.	Sequence	Genus	Species[a]
1	TACGTATGGAGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGTGCGTAGGTGGCAGT GCAAGTCAGATGTGAAAGGCCGGGGCTCAACCCCGGAGCTGCATTTGAAACTGCTCGGC TAGAGTACAGGAGAGGCAGGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCCTGCTGGACTGTTACTGACACTGAGGCACGAAA GCGTGGGGAGCAAACAGG	[Eubacterium] hallii group	*hallii*
2	TACGTATGGAGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGTGCGTAGGTGGCAGT GCAAGTCAGATGTGAAAGGCCGGGGCTCAACCCCGGAGCTGCATTTGAAACTGCATAGC TAGAGTACAGGAGAGGCAGGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCCTGCTGGACTGTTACTGACACTGAGGCACGAAA GCGTGGGGAGCAAACAGG	[Eubacterium] hallii group	*hallii*
3	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGAATG GCAAGTCTGATGTGAAAGGCCGGGGCTCAACCCCGGGACTGCATTGGAAACTGTCAATC TAGAGTACCGGAGGGGTAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	[Ruminococcus] gauvreauii group	NA
4	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGAATG GCAAGTCTGATGTGAAAGGCCGGGGCTCAACCCCGGGACTGCATTGGAAACTGCCAATC TAGAGTACCGGAGGGGTAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	[Ruminococcus] gauvreauii group	NA
5	TACGTATGGTGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGAGTG GCAAGTCTGATGTGAAAACCCGGGGCTCAACCCCGGGACTGCATTGGAAACTGTCAATC TAGAGTACCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	[Ruminococcus] torques group	NA
6	TACGTATGGTGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGCAGGCGGTGCG GCAAGTCTGATGTGAAAGCCCGGGGCTCAACCCCGGTACTGCATTGGAAACTGTCGTAC TAGAGTGTCGGAGGGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGATAACTGACGCTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Agathobacter*	NA
7	TACAGAGGTCTCAAGCGTTGTTCGGAATCACTGGGCGTAAAGCGTGCGTAGGCTGTTTC GTAAGTCGTGTGTGAAAGGCGCGGGCTCAACCCGCGGACGGCACATGATACTGCGAGAC TAGAGTAATGGAGGGGGAACCGGAATTCTCGGTGTAGCAGTGAAATGCGTAGATATCGA GAGGAACACTCGTGGCGAAGGCGGGTTCCTGGACATTAACTGACGCTGAGGCACGAAG GCCAGGGGAGCGAAAGGG	*Akkermansia*	*muciniphila*
8	TACGTAGGGGGCAAGCGTTATCCGGAATTACTGGGTGTAAAGGGTGCGTAGGTGGTATG GCAAGTCAGAAGTGAAAACCCAGGGCTTAACTCTGGGACTGCTTTTGAAACTGTCAGAC TGGAGTGCAGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACATCAGTGGCGAAGGCGGCTTACTGGACTGAAACTGACACTGAGGCACGAAA GCGTGGGGAGCAAACAGG	*Anaerostipes*	*hadrus*
9	TACGTAGGGTGCAAGCGTTATCCGGAATTATTGGGCGTAAAGGGCTCGTAGGCGGTTCG TCGCGTCCGGTGTGAAAGTCCATCGCTTAACGGTGGATCCGCGCCGGGTACGGGCGGGC TTGAGTGCGGTAGGGGAGACTGGAATTCCCGGTGTAACGGTGGAATGTGTAGATATCGG GAAGAACACCAATGGCGAAGGCAGGTCTCTGGGCCGTCACTGACGCTGAGGAGCGAAA GCGTGGGGAGCGAACAGG	*Bifidobacterium*	*adolescentis*
10	TACGTAGGGTGCAAGCGTTATCCGGAATTATTGGGCGTAAAGGGCTCGTAGGCGGTTCG TCGCGTCCGGTGTGAAAGTCCATCGCTTAACGGTGGATCCGCGCCGGGTACGGGCGGGC TTGAGTGCGGTAGGGGAGACTGGAATTCCCGGTGTAACGGTGGAATGTGTAGATATCGG GAAGAACACCAATGGCGAAGGCAGGTCTCTGGGCCGTTACTGACGCTGAGGAGCGAAA GCGTGGGGAGCGAACAGG	*Bifidobacterium*	*breve*
11	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGTGTG GCAAGTCTGATGTGAAAGGCATGGGCTCAACCTGTGGACTGCATTGGAAACTGTCATAC TTGAGTGCCGGAGGGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	*obeum*

Table 2. Non-Certified Top 50 V4 16S rRNA sequences and Genus-Species Identifications (listed alphabetically by genus) in Omnivore Stool

No.	Sequence	Genus	Species[(a)]
12	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGACTG GCAAGTCTGATGTGAAAGGCGGGGGCTCAACCCCTGGACTGCATTGGAAACTGTTAGTC TTGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	*obeum*
13	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGATGG ACAAGTCTGATGTGAAAGGCTGGGGCTCAACCCCGGGACTGCATTGGAAACTGCCCGTC TTGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
14	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCATA ACAAGTCTGATGTGAAAGGCTGGGGCTTAACCCCGGGACTGCATTGGAAACTGTTAAGC TTGAGTGCCGGAGGGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
15	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGATTA GCAAGTCTGATGTGAAAGGCAGGGGCTCAACCCCTGGACTGCATTGGAAACTGCCAGTC TTGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGCAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
16	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCGCA GCAAGTCTGATGTGAAAGGCAGGGGCTTAACCCCTGGACTGCATTGGAAACTGCTGTGC TTGAGTGCCGGAGGGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
17	TACGTAGGTGGCGAGCGTTATCCGGAATCATTGGGCGTAAAGAGGGAGCAGGCGGCCGC AAGGGTCTGTGGTGAAAGACCGAAGCTAAACTTCGGTAAGCCATGGAAACCGGGCGGCT AGAGTGCGGAAGAGGATCGTGGAATTCCATGTGTAGCGGTGAAATGCGTAGATATATGG AGGAACACCAGTGGCGAAGGCGACGGTCTGGGCCGCAACTGACGCTCATTCCCGAAAGC GTGGGGAGCAAATAGG	*Catenibacterium*	NA
18	TACGTAGGTGGCGAGCGTTATCCGGAATCATTGGGCGTAAAGAGGGAGCAGGCGGCCGC AAGGGTCTGTGGTGAAAGACCGAAGCTAAACTTCGGTGAGCCATGGAAACCGGGCGGCT AGAGTGCGGAAGAGGATCGTGGAATTCCATGTGTAGCGGTGAAATGCGTAGATATATGG AGGAACACCAGTGGCGAAGGCGACGGTCTGGGCCGCAACTGACGCTCATTCCCGAAAGC GTGGGGAGCAAATAGG	*Catenibacterium*	NA
19	TACGTAGGTGGCGAGCGTTGTCCGGATTTACTGGGCGTAAAGGGAGCGTAGGCGGATTT TTAAGTGAGATGTGAAATACTCGGGCTTAACCTGAGTGCTGCATTTCAAACTGGAAGTCT AGAGTGCAGGAGAGGAGAAGGGAATTCCTAGTGTAGCGGTGAAATGCGTAGAGATTAG GAAGAACACCAGTGGCGAAGGCGCTTCTCTGGACTGTAACTGACGCTGAGGCTCGAAAG CGTGGGGAGCAAACAGG	*Clostridium sensu stricto 1*	NA
20	TACGTAGGTGGCGAGCGTTGTCCGGATTTACTGGGCGTAAAGGGAGCGTAGGCGGACTT TTAAGTGAGATGTGAAATACCCGGGCTCAACTTGGGTGCTGCATTTCAAACTGGAAGTCT AGAGTGCAGGAGAGGAGAATGGAATTCCTAGTGTAGCGGTGAAATGCGTAGAGATTAG GAAGAACACCAGTGGCGAAGGCGATTCTCTGGACTGTAACTGACGCTGAGGCTCGAAAG CGTGGGGAGCAAACAGG	*Clostridium sensu stricto 1*	NA
21	TACGTAGGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGGCCCG GCAGGCCGGGGGTCGAAGCGGGGGGCTCAACCCCCCGAAGCCCCCGGAACCTCCGCGG CTTGGGTCCGGTAGGGGAGGGTGGAACACCCGGTGTAGCGGTGGAATGCGCAGATATCG GGTGGAACACCGGTGGCGAAGGCGGCCCTCTGGGCCGAGACCGACGCTGAGGCGCGAA AGCTGGGGGAGCGAACAGG	*Collinsella*	*aerofaciens*
22	TACGTAGGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGGCCTG GCAGGCCGGGGGTCAAATGCGGGGGCTCAACCCCCGCCCGCCCCCGGAACCTCCGGGCT TGGGTCCGGTAGGGGAGGGTGGAACACCCGGTGTAGCGGTGGAATGCGCAGATATCGG GTGGAACACCGGTGGCGAAGGCGGCCCTCTGGGCCGTGACCGACGCTGAGGCGCGAAA GCTGGGGGAGCGAACAGG	*Collinsella*	NA
23	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGGCGGCGGA GCAAGTCAGAAGTGAAAGCCCGGGGCTCAACCCCGGGACGGCTTTTGAAACTGCCCTGC TTGATTTCAGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACTGACAATGACGCTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Coprococcus*	*catus*
24	TACGGAGGGTGCAAGCGTTACCCGGAATCACTGGGCGTAAAGGGCGTGTAGGCGGAAA TTTAAGTCTGGTTTTAAAGACCGGGGCTCAACCTCGGGGATGGACTGGATACTGGATTTC TTGACCTCTGGAGAGGTAACTGGAATTCCTGGTGTAGCGGTGGAATGCGTAGATACCAG GAGGAACACCAATGGCGAAGGCAAGTTACTGGACAGAAGGTGACGCTGAGGCGCGAAA GTGTGGGGAGCAAACCGG	*Deinococcus*	*radiodurans*

Table 2. Non-Certified Top 50 V4 16S rRNA sequences and Genus-Species Identifications (listed alphabetically by genus) in Omnivore Stool			
No.	Sequence	Genus	Species[(a)]
25	TACGTAGGGTGCGAGCGTTAATCGGAATTACTGGGCGTAAAGCGTGCGCAGGCGGTTAT GTAAGACAGATGTGAAATCCCCGGGCTCAACCTGGGAACTGCATTTGTGACTGCATGGC TAGAGTACGGTAGAGGGGGATGGAATTCCGCGTGTAGCAGTGAAATGCGTAGATATGCG GAGGAACACCGATGGCGAAGGCAATCCCCTGGACCTGTACTGACGCTCATGCACGAAAG CGTGGGGAGCAAACAGG	*Delftia*	*tsuruhatensis*
26	TACGTAGGTGGCAAGCGTTGTCCGGAATTATTGGGCGTAAAGCGCGCGCAGGCGGCTTC TTAAGTCCATCTTAAAAGTGCGGGGCTTAACCCCGTGATGGGATGGAAACTGAGAGGCT GGAGTATCGGAGAGGAAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGAGATTAG GAAGAACACCGGTGGCGAAGGCGACTTTCTGGACGACAACTGACGCTGAGGCGCGAAA GCGTGGGGAGCAAACAGG	*Dialister*	NA
27	TACGGAGGGTGCAAGCGTTAATCGGAATGACTGGGCGTAAAGCGCACGCAGGCGGTCTG TTAAGTTGGATGTGAAATCCCCGGGCTTAACCTGGGAACTGCATTCAAAACTGACAGGC TAGAGTCTCGTAGAGGGGGGTAGAATTCCAGGTGTAGCGGTGAAATGCGTAGAGATCTG GAGGAATACCGGTGGCGAAGGCGGCCCCCTGGACGAAGACTGACGCTCAGGTGCGAAA GCGTGGGGAGCAAACAGG	*Dickeya*	*zeae*
28	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCACG GCAAGCCAGATGTGAAAGCCCGGGGCTCAACCCCGGGACTGCATTTGGAACTGCTGAGC TAGAGTGTCGGAGAGGCAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTGCTGGACGATGACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Dorea*	NA
29	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCTGT GCAAGTCTGAAGTGAAAGGCATGGGCTCAACCTGTGGACTGCTTTGGAAACTGTGCAGC TAGAGTGTCGGAGAGGTAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGATGACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Dorea*	*formicigenerans*
30	TACGTAGGGGGCGAGCGTTATCCGGAATGATTGGGCGTAAAGCGCGCGCAGGCGGCCGC TCAAGCGGGACCTCTAACCCCGGGGCTCAACCCCGGGCCGGGTCCCGAACTGGGCGGCT CGAGTGCGGTAGGGGAGAGCGGAATTCCAAGTGTAGCGGTGAAATGCGCAGATATTTGG AAGAACACCGATGGCGAAGGCAGCTCTCTGGGCCGTCACTGACGCTGAGGCGCGAAAG CCGGGGGAGCGAACAGG	*Enterorhabdus*	NA
31	TACGTAGGTGGCGAGCGTTATCCGGAATTATTGGGCGTAAAGAGGGAGCAGGCGGCACT AAGGGTCTGTGGTGAAAGATCGAAGCTTAACTTCGGTAAGCCATGGAAACCGTAGAGCT AGAGTGTGTGAGAGGATCGTGGAATTCCATGTGTAGCGGTGAAATGCGTAGATATATGG AGGAACACCAGTGGCGAAGGCGACGATCTGGCGCATAACTGACGCTCAGTCCCGAAAG CGTGGGGAGCAAATAGG	*Erysipelotrichaceae UCG-003*	NA
32	AACGTAGGTCACAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGGAA GACAAGTTGGAAGTGAAATCTATGGGCTCAACCCATAAACTGCTTTCAAAACTGTTTTTC TTGAGTAGTGCAGAGGTAGGCGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCGG GAGGAACACCAGTGGCGAAGGCGGCCTACTGGGCACCAACTGACGCTGAGGCTCGAAA GTGTGGGTAGCAAACAGG	*Faecalibacterium*	*prausnitzii*
33	AACGTAGGTCACAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGGAA GACAAGTTGGAAGTGAAATCCATGGGCTCAACCCATGAACTGCTTTCAAAACTGTTTTTC TTGAGTAGTGCAGAGGTAGGCGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCGG GAGGAACACCAGTGGCGAAGGCGGCCTACTGGGCACCAACTGACGCTGAGGCTCGAAA GTGTGGGTAGCAAACAGG	*Faecalibacterium*	*prausnitzii*
34	TACGTAGGGGGCAAGCGTTATCCGGAATTATTGGGCGTAAAGAGTACGTAGGTGGTTTT CTAAGCACGGGGTTTAAGGCAATGGCTTAACCATTGTTCGCCTTGTGAACTGGAAGACTT GAGTGCAGGAGAGGAAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGG AGGAACACCAGTGGCGAAGGCGGCTTTCTGGACTGTAACTGACACTGAGGTACGAAAGC GTGGGGAGCAAACAGG	*Family XIII AD3011 group*	NA
35	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCAAG GCAAGTCTGATGTGAAAACCCAGGGCTTAACCCTGGGACTGCATTGGAAACTGTCTGGC TCGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAAGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Fusicatenibacter*	NA
36	TACGTAGGTGGCGAGCGTTATCCGGAATGATTGGGCGTAAAGGGTGCGTAGGTGGCAGA TCAAGTCTGGAGTAAAAGGTATGGGCTCAACCCGTACTGGCTCTGGAAACTGATCAGCT AGAGAACAGAAGAGGACGGCGGAACTCCATGTGTAGCGGTAAAATGCGTAGATATATG GAAGAACACCGGTGGCGAAGGCGGCCGTCTGGTCTGGATTCTGACACTGAAGCACGAAA GCGTGGGGAGCAAATAGG	*Holdemanella*	NA
37	TACGTAGGGAGCAAGCGTTGTCCGGATTTACTGGGTGTAAAGGGTGCGTAGGCGGATTG GCAAGTCAGAAGTGAAATCCATGGGCTTAACCCATGAACTGCTTTTGAAACTGTTAGTCT TGAGTGAAGTAGAGGTAGGCGGAATTCCCGGTGTAGCGGTGAAATGCGTAGAGATCGG GAGGAACACCAGTGGCGAAGGCGGCCTACTGGGCTTTAACTGACGCTGAGGCACGAAA GTGTGGGTAGCAAACAGG	*Incertae Sedis*	NA

Table 2. Non-Certified Top 50 V4 16S rRNA sequences and Genus-Species Identifications (listed alphabetically by genus) in Omnivore Stool			
No.	Sequence	Genus	Species[(a)]
38	TACGTAGGTGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGCGTGTAGGCGGGAGT GCAAGTCAGATGTGAAAATTATGGGCTCAACCCATAACCTGCATTTGAAACTGTACTTCT TGAGTACTGGAGAGGCAGGCGGAATTCCGTGTGTAGCGGTGAAATGCGTAGATATACGG AGGAACACCAGTGGCGAAGGCGGCCTGCTGGACAGCAACTGACGCTGAGGCGCGAAAG CGTGGGGAGCAAACAGG	*Intestinimonas*	NA
39	TACGTATGGTGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGGTGGCAAG GCAAGCCAGAAGTGAAAACCCGGGGCTCAACCGCGGGATTGCTTTTGGAACTGTCATGC TAGAGTGCAGGAGGGGTGAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCGGAGGCGAAGGCGGCTCACTGGACTGTAACTGACACTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Lachnospiraceae ND3007 group*	NA
40	TACGTATGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGGCCTG GCAGGCCGGGAGTCAAATCCGGGGGCTCAACCCCCGCCCGCTCCCGGAACCTCCAGGCT TGAGTCTGGCAGGGGAGGGTGGAATACCCGGTGTAGCGGTGGAATGCGCAGATATCGG GTAGAACACCGGTGGCGAAGGCGGCCCTCTGGGCCACGACTGACGCTGAGGCGCGAAA GCTGGGGGAGCGAACAGG	*Libanicoccus*	NA
41	CACCGGCAGCTCTAGTGGTAGCAGTTTTTATTGGGCCTAAAGCGTCCGTAGCCGGTTTAA TAAGTCTCTGGTGAAATCCTGCAGCTTAACTGTGGGAATTGCTGGAGATACTATTAGACT TGAGATCGGGAGAGGTTAGAGGTACTCCCAGGGTAGAGGTGAAATTCTGTAATCCTGGG AGGACCGCCTGTTGCGAAGGCGTCTGACTGGAACGATTCTGACGGTGAGGGACGAAAGC TAGGGGCGCGAACCGG	*Methanobrevibacter*	*smithii*
42	TACGTAGGGGGCAAGCGTTATCCGGAATTATTGGGCGTAAAGAGTGCGTAGGTGGTTAT CTAAGCGTAAGGTTTAAGCGTGCAGCTCAACTGCATCTCGCCTTGCGAACTGGACTACTT GAGTGCAGGAGGGGAAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGG AGGAACACCAGCGGCGAAGGCGGCTTTCTGGACTGTAACTGACACTGAGGCACGAAAG CGTGGGGAGCAAACAGG	*Mogibacterium*	NA
43	TACGTAGGTGACAAGCGTTGTCCGGATTTACTGGGTGTAAAGGGCGCGTAGGCGGACTG TCAAGTCAGTCGTGAAATACCGGGGCTTAACCCCGGGGCTGCGATTGAAACTGACAGCC TTGAGTATCGGAGAGGAAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTTCTGGACGACAACTGACGCTGAGGCGCGAAA GTGTGGGGAGCAAACAGG	*Monoglobus*	NA
44	TACGTAGGGGGCTAGCGTTATCCGGAATTACTGGGCGTAAAGGGTGCGTAGGTGGTTTC TTAAGTCAGAGGTGAAAGGCTACGGCTCAACCGTAGTAAGCCTTTGAAACTGGGAAACT TGAGTGCAGGAGAGGAGAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGG AGGAACACCAGTTGCGAAGGCGGCTCTCTGGACTGTAACTGACACTGAGGCACGAAAGC GTGGGGAGCAAACAGG	*Romboutsia*	*ilealis*
45	TACGTAGGGAGCAAGCGTTGTCCGGATTTACTGGGTGTAAAGGGTGCGTAGGCGGCTTT GCAAGTCAGATGTGAAATCTATGGGCTCAACCCATAAACTGCATTTGAAACTGTAGAGC TTGAGTGAAGTAGAGGCAGGCGGAATTCCCCGTGTAGCGGTGAAATGCGTAGAGATGGG GAGGAACACCAGTGGCGAAGGCGGCCTGCTGGGCTTTAACTGACGCTGAGGCACGAAA GCGTGGGTAGCAAACAGG	*Ruminococcus*	*bromii*
46	TACGTATGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGGAGCG CTAAGCGGGACCTCTAACCCGAGGGCTCAACCCCCGGCCGGGTCCCGAACTGGCGCTCT CGAGTGCGGTAGGGGAGAGCGGAATTCCCGGTGTAGCGGTGGAATGCGCAGATATCGG GAAGAACACCGACGGCGAAGGCAGCTCTCTGGGCCGAAACTGACGCTGAGGCGCGAAA GCTGGGGGAGCGAACAGG	*Senegalimassilia*	NA
47	TACGTAGGTCCCGAGCGTTGTCCGGATTTATTGGGCGTAAAGCGAGCGCAGGCGGTTTG ATAAGTCTGAAGTTAAAGGCTGTGGCTCAACCATAGTTCGCTTTGGAAACTGTCAAACTT GAGTGCAGAAGGGGAGAGTGGAATTCCATGTGTAGCGGTGAAATGCGTAGATATATGG AGGAACACCGGTGGCGAAAGCGGCTCTCTGGTCTGTAACTGACGCTGAGGCTCGAAAGC GTGGGGAGCGAACAGG	*Streptococcus*	*salivarius*
48	AACGTAGGGTGCAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGGAA GACAAGTTGGAAGTGAAAACCATGGGCTCAACCCATGAATTGCTTTCAAAACTGTTTTTC TTGAGTAGTGCAGAGGTAGATGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCGG GAGGAACACCAGTGGCGAAGGCGGTCTACTGGGCACCAACTGACGCTGAGGCTCGAAA GCATGGGTAGCAAACAGG	*Subdoligranulum*	NA
49	AACGTAGGGTGCAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGACC GGCAAGTTGGAAGTGAAAACTATGGGCTCAACCCATAAATTGCTTTCAAAACTGCTGGC CTTGAGTAGTGCAGAGGTAGGTGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCG GGAGGAACACCAGTGGCGAAGGCGACCTACTGGGCACCAACTGACGCTGAGGCTCGAA AGCATGGGTAGCAAACAGG	*Subdoligranulum*	NA
50	TACGTAGGTGGCAAGCGTTGTCCGGATTTACTGGGTGTAAAGGGCGTGTAGCCGGGAAG GCAAGTCAGATGTGAAATCCACGGGCTTAACTCGTGAACTGCATTTGAAACTGTTTTTCT TGAGTATCGGAGAGGCAATCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGG AGGAACACCAGTGGCGAAGGCGGATTGCTGGACGACAACTGACGGTGAGGCGCGAAAG CGTGGGGAGCAAACAGG	UCG-002	NA

[(a)] NA indicates a species was not assigned.

Table 3. Non-Certified Top 50 V4 16S rRNA sequences and Genus-Species Identifications (listed alphabetically by genus) in Vegetarian Stool			
No.	Sequence	Genus	Species[(a)]
1	TACGTATGGAGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGTGCGTAGGTGGCAGTGCAAGTCAGATGTGAAAGGCCGGGGCTCAACCCCGGAGCTGCATTTGAAACTGCTCGGCTAGAGTACAGGAGAGGCAGGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCAGTGGCGAAGGCGGCCTGCTGGACTGTTACTGACACTGAGGCACGAAAGCGTGGGGAGCAAACAGG	[Eubacterium] hallii group	*hallii*
2	TACGTATGGAGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGTGCGTAGGTGGCAGTGCAAGTCAGATGTGAAAGGCCGGGGCTCAACCCCGGAGCTGCATTTGAAACTGCATAGCTAGAGTACAGGAGAGGCAGGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCAGTGGCGAAGGCGGCCTGCTGGACTGTTACTGACACTGAGGCACGAAAGCGTGGGGAGCAAACAGG	[Eubacterium] hallii group	*hallii*
3	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGAATGGCAAGTCTGATGTGAAAGGCCGGGGCTCAACCCCGGGACTGCATTGGAAACTGTCAATCTAGAGTACCGGAGGGGTAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAAGCGTGGGGAGCAAACAGG	[Ruminococcus] gauvreauii group	NA
4	TACGTATGGTGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGAGTGGCAAGTCTGATGTGAAAACCCGGGGCTCAACCCCGGGACTGCATTGGAAACTGTCAATCTAGAGTACCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAAGCGTGGGGAGCAAACAGG	[Ruminococcus] torques group	NA
5	TACGTAGGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGGCCGCCTAAGCGGAACCTCTAATCCCGGGGCTCAACCTCGGGCCGGGTTCCGGACTGGGCGGCTCGAGTGCGGTAGAGGCAGGCGGAATTCCCGGTGTAGCGGTGGAATGCGCAGATATCGGGAAGAACACCGATGGCGAAGGCAGCCTGCTGGGCCGCCACTGACGCTGAGGCGCGAAAGCTGGGGGAGCGAACAGG	*Adlercreutzia*	NA
6	TACGTATGGTGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGCAGGCGGTGCGGCAAGTCTGATGTGAAAGCCCGGGGCTCAACCCCGGTACTGCATTGGAAACTGTCGTACTAGAGTGTCGGAGGGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGATAACTGACGCTGAGGCTCGAAAGCGTGGGGAGCAAACAGG	*Agathobacter*	NA
7	TACAGAGGTCTCAAGCGTTGTTCGGAATCACTGGGCGTAAAGCGTGCGTAGGCTGTTTCGTAAGTCGTGTGTGAAAGGCGCGGGCTCAACCCGCGGACGGCACATGATACTGCGAGACTAGAGTAATGGAGGGGGAACCGGAATTCTCGGTGTAGCAGTGAAATGCGTAGATATCGAGAGGAACACTCGTGGCGAAGGCGGGTTCCTGGACATTAACTGACGCTGAGGCACGAAGGCCAGGGGAGCGAAAGGG	*Akkermansia*	*muciniphila*
8	TACGTAGGGGGCAAGCGTTATCCGGAATTACTGGGTGTAAAGGGTGCGTAGGTGGTATGGCAAGTCAGAAGTGAAAACCCAGGGCTTAACTCTGGGACTGCTTTTGAAACTGTCAGACTGGAGTGCAGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACATCAGTGGCGAAGGCGGCTTACTGGACTGAAACTGACACTGAGGCACGAAAGCGTGGGGAGCAAACAGG	*Anaerostipes*	*hadrus*
9	TACGTAGGGGGCAAGCGTTATCCGGAATTACTGGGTGTAAAGGGTGCGTAGGTGGTATGGCAAGTCAGAAGTGAAAACCCAGGGCTTAACTCTGGGACTGCTTTTGAAACTGTCAGACTAGAGTGCAGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACATCAGTGGCGAAGGCGGCTTACTGGACTGAAACTGACACTGAGGCACGAAAGCGTGGGGAGCAAACAGG	*Anaerostipes*	*hadrus*
10	TACGTAGGGTGCAAGCGTTATCCGGAATTATTGGGCGTAAAGGGCTCGTAGGCGGTTCGTCGCGTCCGGTGTGAAAGTCCATCGCTTAACGGTGGATCCGCGCCGGGTACGGGCGGGCTTGAGTGCGGTAGGGGAGACTGGAATTCCCGGTGTAACGGTGGAATGTGTAGATATCGGGAAGAACACCAATGGCGAAGGCAGGTCTCTGGGCCGTCACTGACGCTGAGGAGCGAAAGCGTGGGGAGCGAACAGG	*Bifidobacterium*	*adolescentis*
11	TACGTAGGGTGCAAGCGTTATCCGGAATTATTGGGCGTAAAGGGCTCGTAGGCGGTTCGTCGCGTCCGGTGTGAAAGTCCATCGCTTAACGGTGGATCCGCGCCGGGTACGGGCGGGCTTGAGTGCGGTAGGGGAGACTGGAATTCCCGGTGTAACGGTGGAATGTGTAGATATCGGGAAGAACACCAATGGCGAAGGCAGGTCTCTGGGCCGTTACTGACGCTGAGGAGCGAAAGCGTGGGGAGCGAACAGG	*Bifidobacterium*	*breve*
12	TACGTAGGGTGCGAGCGTTATCCGGATTTATTGGGCGTAAAGGGCTCGTAGGCGGTTCGTCGCGTCCGGTGTGAAAGTCCATCGCCTAACGGTGGATCTGCGCCGGGTACGGGCGGGCTGGAGTGCGGTAGGGGAGACTGGAATTCCCGGTGTAACGGTGGAATGTGTAGATATCGGGAAGAACACCAATGGCGAAGGCAGGTCTCTGGGCCGTCACTGACGCTGAGGAGCGAAAGCGTGGGGAGCGAACAGG	*Bifidobacterium*	*animalis*

Table 3. Non-Certified Top 50 V4 16S rRNA sequences and Genus-Species Identifications (listed alphabetically by genus) in Vegetarian Stool			
No.	Sequence	Genus	Species[a]
13	TACGTAGGGTGCAAGCGTTATCCGGAATTATTGGGCGTAAAGGGCTCGTAGGCGGTTCG TCGCGTCCGGTGTGAAAGTCCATCGCTTAACGGTGGATCTGCGCCGGGTACGGGCGGGC TGGAGTGCGGTAGGGGAGACTGGAATTCCCGGTGTAACGGTGGAATGTGTAGATATCGG GAAGAACACCAATGGCGAAGGCAGGTCTCTGGGCCGTTACTGACGCTGAGGAGCGAAA GCGTGGGGAGCGAACAGG	*Bifidobacterium*	*catenulatum*
14	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGTGTG GCAAGTCTGATGTGAAAGGCATGGGCTCAACCTGTGGACTGCATTGGAAACTGTCATAC TTGAGTGCCGGAGGGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	*obeum*
15	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGATGG ACAAGTCTGATGTGAAAGGCTGGGGCTCAACCCCGGGACTGCATTGGAAACTGCCCGTC TTGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
16	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGACTG GCAAGTCTGATGTGAAAGGCGGGGGCTCAACCCCTGGACTGCATTGGAAACTGTTAGTC TTGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	*obeum*
17	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCGCA GCAAGTCTGATGTGAAAGGCAGGGGCTTAACCCCTGGACTGCATTGGAAACTGCTGTGC TTGAGTGCCGGAGGGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
18	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGAGCA GCAAGTCTGATGTGAAAGGCGGGGGCTCAACCCCCGGACTGCATTGGAAACTGTTGATC TTGAGTACCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
19	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGATTA GCAAGTCTGATGTGAAAGGCAGGGGCTCAACCCCTGGACTGCATTGGAAACTGCCAGTC TTGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGCAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
20	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGTGTT GCAAGTCTGATGTGAAAGGCGGGGGCTCAACCCCTGGACTGCATTGGAAACTGTGATAC TCGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Blautia*	NA
21	TACGTAGGGAGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGCGCGCAGGCGGGCCG GTAAGTTGGAAGTGAAATCTATGGGCTTAACCCATAAACTGCTTTCAAAACTGCTGGTCT TGAGTGATGGAGAGGCAGGCGGAATTCCGTGTGTAGCGGTGAAATGCGTAGATATACGG AGGAACACCAGTGGCGAAGGCGGCCTGCTGGACATTAACTGACGCTGAGGCGCGAAAG CGTGGGGAGCAAACAGG	*Butyricicoccus*	NA
22	TACGTAGGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGGCCCG GCAGGCCGGGGGTCGAAGCGGGGGGCTCAACCCCCCGAAGCCCCCGGAACCTCCGCGG CTTGGGTCCGGTAGGGGAGGGTGGAACACCCGGTGTAGCGGTGGAATGCGCAGATATCG GGTGGAACACCGGTGGCGAAGGCGGCCCTCTGGGCCGAGACCGACGCTGAGGCGCGAA AGCTGGGGGAGCGAACAGG	*Collinsella*	*aerofaciens*
23	TACGTAGGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGGCCCG GCAGGCAGGGGGTCAAATGGCGGGGCTCAACCCCGTCCCGCCCCCTGAACCGCCGGGCT CGGGTCCGGTAGGGGAGGGTGGAACACCCGGTGTAGCGGTGGAATGCGCAGATATCGG GTGGAACACCGGTGGCGAAGGCGGCCCTCTGGGCCGAGACCGACGCTGAGGCGCGAAA GCTGGGGGAGCGAACAGG	*Collinsella*	*stercoris*
24	TACGTATGGTGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCTGT GTAAGTCTGAAGTGAAAGCCCGGGGCTCAACCCCGGGACTGCTTTGGAAACTATGCAGC TAGAGTGTCGGAGAGGTAAGTGGAATTCCCAGTGTAGCGGTGAAATGCGTAGATATTGG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGATGACTGACGTTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Coprococcus*	*comes*
25	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGGCGGCGGA GCAAGTCAGAAGTGAAAGCCCGGGGCTCAACCCCGGGACGGCTTTTGAAACTGCCCTGC TTGATTTCAGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTACTGGACTGACAATGACGCTGAGGCTCGAAA GCGTGGGGAGCAAACAGG	*Coprococcus*	*catus*

Table 3. Non-Certified Top 50 V4 16S rRNA sequences and Genus-Species Identifications (listed alphabetically by genus) in Vegetarian Stool			
No.	Sequence	Genus	Species[a]
26	TACGGAGGGTGCAAGCGTTACCCGGAATCACTGGGCGTAAAGGGCGTGTAGGCGGAAATTTAAGTCTGGTTTTAAAGACCGGGGCTCAACCTCGGGGATGGACTGGATACTGGATTTCTTGACCTCTGGAGAGGTAACTGGAATTCCTGGTGTAGCGGTGGAATGCGTAGATACCAGGAGGAACACCAATGGCGAAGGCAAGTTACTGGACAGAAGGTGACGCTGAGGCGCGAAAGTGTGGGGAGCAAACCGG	*Deinococcus*	*radiodurans*
27	TACGTAGGGTGCGAGCGTTAATCGGAATTACTGGGCGTAAAGCGTGCGCAGGCGGTTATGTAAGACAGATGTGAAATCCCCGGGCTCAACCTGGGAACTGCATTTGTGACTGCATGGCTAGAGTACGGTAGAGGGGGATGGAATTCCGCGTGTAGCAGTGAAATGCGTAGATATGCGGAGGAACACCGATGGCGAAGGCAATCCCCTGGACCTGTACTGACGCTCATGCACGAAAGCGTGGGGAGCAAACAGG	*Delftia*	*tsuruhatensis*
28	TACGTAGGTGGCAAGCGTTGTCCGGAATTATTGGGCGTAAAGCGCGCGCAGGCGGCTTCCCAAGTCCCTCTTAAAAGTGCGGGGCTTAACCCCGTGATGGGAAGGAAACTGGGAAGCTGGAGTATCGGAGAGGAAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGAGATTAGGAAGAACACCGGTGGCGAAGGCGACTTTCTGGACGAAAACTGACGCTGAGGCGCGAAAGCGTGGGGAGCAAACAGG	*Dialister*	*invisus*
29	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCACGGCAAGCCAGATGTGAAAGCCCGGGGCTCAACCCCGGGACTGCATTTGGAACTGCTGAGCTAGAGTGTCGGAGAGGCAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCAGTGGCGAAGGCGGCTTGCTGGACGATGACTGACGTTGAGGCTCGAAAGCGTGGGGAGCAAACAGG	*Dorea*	NA
30	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCTGTGCAAGTCTGAAGTGAAAGGCATGGGCTCAACCTGTGGACTGCTTTGGAAACTGTGCAGCTAGAGTGTCGGAGAGGTAAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCAGTGGCGAAGGCGGCTTACTGGACGATGACTGACGTTGAGGCTCGAAAGCGTGGGGAGCAAACAGG	*Dorea*	*formicigenerans*
31	AACGTAGGTCACAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGGAAGACAAGTTGGAAGTGAAATCTATGGGCTCAACCCATAAACTGCTTTCAAAACTGTTTTTCTTGAGTAGTGCAGAGGTAGGCGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCGGGAGGAACACCAGTGGCGAAGGCGGCCTACTGGGCACCAACTGACGCTGAGGCTCGAAAGTGTGGGTAGCAAACAGG	*Faecalibacterium*	*prausnitzii*
32	AACGTAGGTCACAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGGCGATCAAGTTGGAAGTGAAATCCATGGGCTCAACCCATGAACTGCTTTCAAAACTGATTGTCTTGAGTAGTGCAGAGGTAGGCGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCGGGAGGAACACCAGTGGCGAAGGCGGCCTACTGGGCACCAACTGACGCTGAGGCTCGAAAGTGTGGGTAGCAAACAGG	*Faecalibacterium*	NA
33	AACGTAGGTCACAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGGAAGACAAGTTGGAAGTGAAATCCATGGGCTCAACCCATGAACTGCTTTCAAAACTGTTTTTCTTGAGTAGTGCAGAGGTAGGCGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCGGGAGGAACACCAGTGGCGAAGGCGGCCTACTGGGCACCAACTGACGCTGAGGCTCGAAAGTGTGGGTAGCAAACAGG	*Faecalibacterium*	*prausnitzii*
34	TACGTAGGGGGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGACGGCAAGGCAAGTCTGATGTGAAAACCCAGGGCTTAACCCTGGGACTGCATTGGAAACTGTCTGGCTCGAGTGCCGGAGAGGTAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAAGAACACCAGTGGCGAAGGCGGCTTACTGGACGGTAACTGACGTTGAGGCTCGAAAGCGTGGGGAGCAAACAGG	*Fusicatenibacter*	NA
35	TACGTAGGTGGCGAGCGTTATCCGGAATGATTGGGCGTAAAGGGTGCGTAGGTGGCAGATCAAGTCTGGAGTAAAAGGTATGGGCTCAACCCGTACTGGCTCTGGAAACTGATCAGCTAGAGAACAGAAGAGGACGGCGGAACTCCATGTGTAGCGGTAAAATGCGTAGATATATGGAAGAACACCGGTGGCGAAGGCGGCCGTCTGGTCTGGATTCTGACACTGAAGCACGAAAGCGTGGGGAGCAAATAGG	*Holdemanella*	NA
36	TACGTAGGGAGCAAGCGTTGTCCGGATTTACTGGGTGTAAAGGGTGCGTAGGCGGATTGGCAAGTCAGAAGTGAAATCCATGGGCTTAACCCATGAACTGCTTTGAAACTGTTAGTCTTGAGTGAAGTAGAGGTAGGCGGAATTCCCGGTGTAGCGGTGAAATGCGTAGAGATCGGGAGGAACACCAGTGGCGAAGGCGGCCTACTGGGCTTTAACTGACGCTGAGGCACGAAAGTGTGGGTAGCAAACAGG	*Incertae Sedis*	NA
37	TACGTATGGTGCAAGCGTTATCCGGATTTACTGGGTGTAAAGGGAGCGTAGGTGGCAAGGCAAGCCAGAAGTGAAAACCCGGGGCTCAACCGCGGGATTGCTTTTGGAACTGTCATGCTAGAGTGCAGGAGGGGTGAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGGAGGAACACCGGAGGCGAAGGCGGCTCACTGGACTGTAACTGACACTGAGGCTCGAAAGCGTGGGGAGCAAACAGG	*Lachnospiraceae ND3007 group*	NA
38	TACGTAGGTGGCAAGCGTTATCCGGATTTATTGGGCGTAAAGCGAGCGCAGGCGGTTTGATAAGTCTGATGTGAAAGCCTTTGGCTTAACCAAAGAAGTGCATCGGAAACTGTCAGACTTGAGTGCAGAAGAGGACAGTGGAACTCCATGTGTAGCGGTGGAATGCGTAGATATATGGAAGAACACCAGTGGCGAAGGCGGCTGTCTGGTCTGCAACTGACGCTGAGGCTCGAAAGCATGGGTAGCGAACAGG	*Lactobacillus*	*mucosae*

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No.	Sequence	Genus	Species[a]
39	TACGTAGGCGGCAAGCGTTGTCCGGAATTATTGGGCGTAAAGGGAGCGCAGGCGGGAA ACTAAGCGGATCTTAAAAGTGCGGGGCTCAACCCCGTGATGGGGTCCGAACTGGTTTTC TTGAGTGCAGGAGAGGAAAGCGGAATTCCCAGTGTAGCGGTGAAATGCGTAGATATTGG GAAGAACACCAGTGGCGAAGGCGGCTTTCTGGACTGTAACTGACGCTGAGGCTCGAAAG CTAGGGTAGCGAACGGG	*Megamonas*	NA
40	CACCGGCAGCTCTAGTGGTAGCAGTTTTTATTGGGCCTAAAGCGTCCGTAGCCGGTTTAA TAAGTCTCTGGTGAAATCCTGCAGCTTAACTGTGGGAATTGCTGGAGATACTATTAGACT TGAGATCGGGAGAGGTTAGAGGTACTCCCAGGGTAGAGGTGAAATTCTGTAATCCTGGG AGGACCGCCTGTTGCGAAGGCGTCTGACTGGAACGATTCTGACGGTGAGGGACGAAAGC TAGGGGCGCGAACCGG	*Methanobrevibacter*	*smithii*
41	CACCGGCAGCTCAAGTGGTAGCTGTTTTTATTGGGCCTAAAGCGTTCGTAGCCGGTTTGA TAAGTCTTTGGTGAAAGCTTGTAGCTTAACTATAAGAATTGCTGAAGATACTGTCAGACT TGAAGTCGGGAGAGGTTAGAGGTACTACCGGGGTAGGGGTGAAATCCTATAATCCTGGG AGGACCACCTGTGGCGAAGGCGTCTAACTGGAACGATCTTGACGGTGAGTAACGAAAGC CAGGGGCGCGAACCGG	*Methanosphaera*	*stadtmanae*
42	TACGTAGGTGACAAGCGTTGTCCGGATTTACTGGGTGTAAAGGGCGCGTAGGCGGACTG TCAAGTCAGTCGTGAAATACCGGGGCTTAACCCCGGGGCTGCGATTGAAACTGACAGCC TTGAGTATCGGAGAGGAAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTTCTGGACGACAACTGACGCTGAGGCGCGAAA GTGTGGGGAGCAAACAGG	*Monoglobus*	NA
43	TACGTAGGTGGCAAGCGTTGTCCGGATTTACTGGGTGTAAAGGGCGTGTAGGCGGGTAG ACAAGTCAGATGTGAAATACCGGGGCTCAACTCCGGGGCTGCATTTGAAACTGTATATC TTGAGTGTCGGAGAGGAAAGCGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAG GAGGAACACCAGTGGCGAAGGCGGCTTTCTGGACGATAACTGACGCTGAGGCGCGAAA GCGTGGGGAGCAAACAGG	*Monoglobus*	*pectinilyticus*
44	TACGTAGGGGGCTAGCGTTATCCGGATTTACTGGGCGTAAAGGGTGCGTAGGCGGTCTT TCAAGTCAGGAGTTAAAGGCTACGGCTCAACCGTAGTAAGCTCCTGATACTGTCTGACTT GAGTGCAGGAGAGGAAAGCGGAATTCCCAGTGTAGCGGTGAAATGCGTAGATATTGGG AGGAACACCAGTAGCGAAGGCGGCTTTCTGGACTGTAACTGACGCTGAGGCACGAAAGC GTGGGGAGCAAACAGG	*Peptoclostridium*	NA
45	TACGTAGGTGGCGAGCGTTGTCCGGAATTATTGGGCGTAAAGAGCATGTAGGCGGCTTA ATAAGTCGAGCGTGAAAATGCGGGGCTCAACCCCGTATGGCGCTGGAAACTGTTAGGCT TGAGTGCAGGAGAGGAAAGGGGAATTCCCAGTGTAGCGGTGAAATGCGTAGATATTGG GAGGAACACCAGTGGCGAAGGCGCCTTTCTGGACTGTGTCTGACGCTGAGATGCGAAAG CCAGGGTAGCGAACGGG	*Phascolarctobacteri um*	*faecium*
46	TACGTAGGGGGCTAGCGTTATCCGGAATTACTGGGCGTAAAGGGTGCGTAGGTGGTTTC TTAAGTCAGAGGTGAAAGGCTACGGCTCAACCGTAGTAAGCCTTTGAAACTGGGAAACT TGAGTGCAGGAGAGGAGAGTGGAATTCCTAGTGTAGCGGTGAAATGCGTAGATATTAGG AGGAACACCAGTTGCGAAGGCGGCTCTCTGGACTGTAACTGACACTGAGGCACGAAAGC GTGGGGAGCAAACAGG	*Romboutsia*	*ilealis*
47	TACGTAGGGGGCGAGCGTTATCCGGATTCATTGGGCGTAAAGCGCGCGTAGGCGTCCCT TCAAGCGGCACCGTCGAAGCCGGGGGCTCAACCCCCGGAAGCGGGCCGAACTGGGGGG ATCGAGTGCGGTAGGGGAAGGCGGAATTCCCGGTGTAGCGGTGAAATGCGCAGATATCG GGAAGAACACCGACGGCGAAGGCAGCCTTCTGGGCCGCCACTGACGCTGAGGCGCGAA AGCTGGGGGAGCGAACAGG	*Slackia*	*piriformis*
48	TACGTAGGTCCCGAGCGTTGTCCGGATTTATTGGGCGTAAAGCGAGCGCAGGCGGTTTG ATAAGTCTGAAGTTAAAGGCTGTGGCTCAACCATAGTTCGCTTTGGAAACTGTCAAACTT GAGTGCAGAAGGGGAGAGTGGAATTCCATGTGTAGCGGTGAAATGCGTAGATATATGG AGGAACACCGGTGGCGAAAGCGGCTCTCTGGTCTGTAACTGACGCTGAGGCTCGAAAGC GTGGGGAGCGAACAGG	*Streptococcus*	*salivarius*
49	AACGTAGGGTGCAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGGAA GACAAGTTGGAAGTGAAAACCATGGGCTCAACCCATGAATTGCTTTCAAAACTGTTTTTC TTGAGTAGTGCAGAGGTAGATGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCGG GAGGAACACCAGTGGCGAAGGCGGTCTACTGGGCACCAACTGACGCTGAGGCTCGAAA GCATGGGTAGCAAACAGG	*Subdoligranulum*	NA
50	AACGTAGGGTGCAAGCGTTGTCCGGAATTACTGGGTGTAAAGGGAGCGCAGGCGGACC GGCAAGTTGGAAGTGAAAACTATGGGCTCAACCCATAAATTGCTTTCAAAACTGCTGGC CTTGAGTAGTGCAGAGGTAGGTGGAATTCCCGGTGTAGCGGTGGAATGCGTAGATATCG GGAGGAACACCAGTGGCGAAGGCGACCTACTGGGCACCAACTGACGCTGAGGCTCGAA AGCATGGGTAGCAAACAGG	*Subdoligranulum*	NA

[a] NA indicates a species was not assigned.

Table 4. Non-Certified Metabolite Identifications of Omnivore Stool by LC-MS/MS	
Metabolite ID	InChiKey
(1-Ethoxy-1-oxo-4-phenylbutan-2-yl)alanine	CEIWXEQZZZHLDM-UHFFFAOYSA-N
(2E,4E,6E)-11-(1,3-Benzodioxol-5-yl)-N-(2-methylpropyl)undeca-2,4,6-trienamide	ITXVWRWWWSDXOY-HNZFQPFYSA-N
(2S)-2-[(3-Methylbutanoyl)amino]pentanedioic acid	HCVIJONZMYVLAW-ZETCQYMHSA-N
(3-beta)-Allopregnanolone sulfate	MENQCIVHHONJLU-FZCSVUEKSA-N
(4-Methylphenyl)oxidanesulfonic acid	WGNAKZGUSRVWRH-UHFFFAOYSA-N
1,2-Di-(9Z,12Z,15Z-octadecatrienoyl)-sn-glycero-3-phosphocholine	XXKFQTJOJZELMD-JICBSJGISA-N
1,2-Dioctadecanoyl-sn-glycerol	UHUSDOQQWJGJQS-QNGWXLTQSA-N
1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine-N,N-dimethyl	XHPZRQBHFOVLEJ-UNUIOPIBSA-N
1,2-Dioleoyl-sn-glycerol	AFSHUZFNMVJNKX-LLWMBOQKSA-N
1,2-Dipalmitoyl-sn-glycero-3-phosphoethanolamine	SLKDGVPOSSLUAI-PGUFJCEWSA-N
1,2-Dipalmitoyl-sn-glycero-O-ethyl-3-phosphatidylcholine cation	VBZSUWNESITEBV-KHBQWKRXSA-N
1,2-Dipentadecanoyl-sn-glycero-3-phosphocholine	LJARBVLDSOWRJT-PSXMRANNSA-N
1,2-Dipentadecanoyl-sn-glycero-3-phosphoethanolamine	SKVKIGSFTGVBOX-MGBGTMOVSA-N
1,3,7-Trimethyluric acid	BYXCFUMGEBZDDI-UHFFFAOYSA-N
1,4-Anhydro-6-O-[(9Z)-9-octadecenoyl]-D-glucitol	NWGKJDSIEKMTRX-AAZCQSIUSA-N
1,6-Hexamethylene-bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]	ZVVFVKJZNVSANF-UHFFFAOYSA-N
1,7-Dimethyluric acid	NOFNCLGCUJJPKU-UHFFFAOYSA-N
13(S)-HOTrE	KLLGGGQNRTVBSU-FQSPHKRJSA-N
13-Keto-9Z,11E-octadecadienoic acid	JHXAZBBVQSRKJR-BSZOFBHHSA-N
14-(acetyloxy)-6-(furan-3-yl)-12-hydroxy-1,7,11,15,15-pentamethyl-5-oxo-3-oxapentacyclo[8.8.0.02,4.02,7.011,16]octadecan-18-yl acetate	PVCLMZBWMWIHKX-UHFFFAOYSA-N
1a,1b-Dihomo prostaglandin E1	YMDDELUTDBQEMT-QZCLESEGSA-N
1-Behenoyl-2-hydroxy-sn-glycero-3-phosphocholine	UIINDYGXBHJQHX-GDLZYMKVSA-N
1-Dodecyl-2-pyrrolidinone	NJPQAIBZIHNJDO-UHFFFAOYSA-N
1-Hexadecyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine	DUUSFCFZBREELS-LXDDVLOTSA-N
1-Hexadecyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine	SIEDNCDNGMIKST-IYEJTHTFSA-N
1-Isopropyl-5-oxo-3-pyrrolidinecarboxylic acid	YKWIPHFVESIOGN-UHFFFAOYSA-N
1-Monolinolenin	GGJRAQULURVTAJ-PDBXOOCHSA-N
1-Monolinoleoyl-rac-glycerol	WECGLUPZRHILCT-HZJYTTRNSA-N
1-Myristoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	RPXHXZNGZBHSMJ-GOSISDBHSA-N
1-Oleoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol)	FQQQKGAFQIIGLQ-VYFUBJQISA-N
1-Oleoyl-2-linoleoyl-rac-glycerol	BLZVZPYMHLXLHG-RQOIEFAZSA-N
1-O-Octadecyl-sn-glyceryl-3-phosphorylcholine	XKBJVQHMEXMFDZ-AREMUKBSSA-N
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	YVYMBNSKXOXSKW-HXUWFJFHSA-N
1-Palmitoyl-2-linoleoyl-rac-glycerol	SVXWJFFKLMLOHO-BCTRXSSUSA-N
1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine	JLPULHDHAOZNQI-ZTIMHPMXSA-N
1-Palmitoyl-2-myristoyl-sn-glycero-3-phosphocholine	UIXXHROAQSBBOV-PSXMRANNSA-N
1-Palmitoyl-2-oleoyl-sn-glycerol	YEJYLHKQOBOSCP-OZKTZCCCSA-N
1-Palmitoyl-3-oleoyl-sn-glycero-2-phosphoethanolamine	BLMYNJDXEOSYBR-OTMQOFQLSA-N
1-Palmitoyl-sn-glycero-3-phosphocholine	ASWBNKHCZGQVJV-HSZRJFAPSA-N
1-Pentadecanoyl-sn-glycero-3-phosphocholine	RJZVWDTYEWCUAR-JOCHJYFZSA-N
1-Stearoyl-2-arachidonyl-sn-glycero-3-phosphocholine	PSVRFUPOQYJOOZ-RYIOQAQXSA-N
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine	IHNKQIMGVNPMTC-RUZDIDTESA-N
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	BBYWOYAFBUOUFP-JOCHJYFZSA-N

Table 4. Non-Certified Metabolite Identifications of Omnivore Stool by LC-MS/MS

Metabolite ID	InChiKey
1-Stearoyl-2-oleoyl-sn-glycero-3-phosphocholine	ATHVAWFAEPLPPQ-VRDBWYNSSA-N
1-Stearoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine	JQKOHRZNEOQNJE-DJEJVYNPSA-N
2-((3aR,4S,7R,7aS)-1,3-Dioxohexahydro-1H-4,7-methanoisoindol-2(3H)-yl)propanoic acid	REFMTLIXGKZVDF-RQOWMOBWSA-N
2-(14,15-Epoxyeicosatrienoyl) glycerol	LPMVKZXODWQHGJ-ILYOTBPNSA-N
2-(1-Methyl-1H-pyrrol-2-yl)acetic acid	SYYOUHJJSOLSJD-UHFFFAOYSA-N
2-(Hexadecylamino)ethanol	SIFHZKKXWMJWOB-UHFFFAOYSA-N
2-(O-beta-D-Glucopyranosyl)atractyligenin	ZUDBDCBPZHGAEL-ICRASABDSA-N
2,3,4,9-Tetrahydro-1H-beta-carboline-3-carboxylic acid	FSNCEEGOMTYXKY-UHFFFAOYSA-N
2,3-Dihydroxypropyl octadecanoate	VBICKXHEKHSIBG-UHFFFAOYSA-N
2,4-Bis(1,1-dimethylethyl)phenol phosphate	GUDSEWUOWPVZPC-UHFFFAOYSA-N
2-[(2R,4aS,8S,8aS)-8-{2-[(4aS,7R,8aR)-7-(1-Carboxyvinyl)-1-hydroxy-4a-methyl-2-oxo-1,2,4a,5,6,7,8,8a-octahydro-1-naphthalenyl]ethyl}-4a-methyl-7-oxo-1,2,3,4,4a,7,8,8a-octahydro-2-naphthalenyl]acrylic acid	BSSWIRVAMSGQMG-RTTXQYISSA-N
2-[(3R,4S)-3-{[5-(Cyclohexylmethyl)-1,2-oxazol-3-yl]methyl}-4-piperidinyl]-N-[2-(4-morpholinyl)ethyl]acetamide	CBYSOGZECVBHQN-SFTDATJTSA-N
2-Arachidonoyl glycerol	RCRCTBLIHCHWDZ-DOFZRALJSA-N
2'-Deoxyadenosine	OLXZPDWKRNYJJZ-RRKCRQDMSA-N
2'-Deoxyinosine	VGONTNSXDCQUGY-JXBXZBNISA-N
2-Linoleoyl-1-palmitoyl-sn-glycero-3-phosphoethanolamine	HBZNVZIRJWODIB-NHCUFCNUSA-N
2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine	WTJKGGKOPKCXLL-VYOBOKEXSA-N
2-Palmitoyl-rac-glycerol	BBNYCLAREVXOSG-UHFFFAOYSA-N
3-(1H-Imidazol-4-yl)propanoic acid	ZCKYOWGFRHAZIQ-UHFFFAOYSA-N
3,4-Dihydroxyhydrocinnamic acid	DZAUWHJDUNRCTF-UHFFFAOYSA-N
3-[5-(2-Methylpropyl)-3,6-dioxopiperazin-2-yl]propanoic acid	CSRXCVLPMJBQIM-UHFFFAOYSA-N
3-beta-Hydroxy-5-cholestenoic acid	WVXOMPRLWLXFAP-AMQKJUDNSA-N
3-Hydroxybutyric acid	WHBMMWSBFZVSSR-UHFFFAOYSA-N
3-Hydroxymyristic acid	ATRNZOYKSNPPBF-UHFFFAOYSA-N
3-Hydroxypyridine	GRFNBEZIAWKNCO-UHFFFAOYSA-N
3-Hydroxyurs-12-en-23-oic acid	NBGQZFQREPIKMG-UHFFFAOYSA-N
3-Sulfopropanoic acid	OURSFPZPOXNNKX-UHFFFAOYSA-N
4,4-Dimethylcholest-8(9),24-dien-3.beta.-ol	CHGIKSSZNBCNDW-QGBOJXOESA-N
4-Cholestenone	NYOXRYYXRWJDKP-GYKMGIIDSA-N
4-Hydroxyomeprazole sulfide	LVUFHVGKGMRSQW-UHFFFAOYSA-N
4-Pyridoxic acid	HXACOUQIXZGNBF-UHFFFAOYSA-N
5-(Dimethylamino)pentanoic acid	UYZSNVLEDLCWGU-UHFFFAOYSA-N
5-[(10Z)-14-(3,5-dihydroxyphenyl)tetradec-10-en-1-yl]benzene-1,3-diol	PFIQXUYXVYYERO-ALCCZGGFSA-N
5-Acetylamino-6-amino-3-methyluracil	POQOTWQIYYNXAT-UHFFFAOYSA-N
5-Hydroxyindole-3-acetic acid	DUUGKQCEGZLZNO-UHFFFAOYSA-N
5-O-Feruloylquinic acid	RAGZUCNPTLULOL-KQJPBSFVSA-N
5-Oxotetrahydro-2-furancarboxylic acid	QVADRSWDTZDDGR-UHFFFAOYSA-N
6-Cyclopentacycloundecenecarboxylic acid, 1,2,3,3a,4,5,6,7,8,9,12,12a-dodecahydro-3a,10-dimethyl-1-(1-methylethenyl)-	FVDVQQJLECWRKH-NVNXTCNLSA-N
6-Methyl-1,2,3-oxathiazin-4(3H)-one 2,2-dioxide	YGCFIWIQZPHFLU-UHFFFAOYSA-N
8-(3-Octyl-2-oxiranyl)octanoic acid	IMYZYCNQZDBZBQ-UHFFFAOYSA-N
9-Nitrooleate	CQOAKBVRRVHWKV-SAPNQHFASA-N
Allyl 4-amino-1-piperidinecarboxylate	XKLGRJGBMKOQDK-UHFFFAOYSA-N

Table 4. Non-Certified Metabolite Identifications of Omnivore Stool by LC-MS/MS	
Metabolite ID	InChiKey
alpha,alpha-Dilaurin	KUVAEMGNHJQSMH-UHFFFAOYSA-N
alpha-Hyodeoxycholic acid methyl ester	BWDRDVHYVJQWBO-QWXHOCAMSA-N
alpha-Tocopheryl acetate	ZAKOWWREFLAJOT-PDNQPUDYSA-N
Anacardic acid	ADFWQBGTDJIESE-UHFFFAOYSA-N
Aspartic acid	CKLJMWTZIZZHCS-UHFFFAOYSA-N
Asp-Pro	UKGGPJNBONZZCM-WDSKDSINSA-N
Bacilysocin	DIGHTWUQPWHBPG-UHFFFAOYSA-N
Benzenesulfonic acid, 4-(acetylamino)-	ZQPVMSLLKQTRMG-UHFFFAOYSA-N
Benzyldimethyldodecylammonium cation	CYDRXTMLKJDRQH-UHFFFAOYSA-N
Benzyldimethylstearylammonium cation	FWLORMQUOWCQPO-UHFFFAOYSA-N
beta-Hyodeoxycholic acid	DGABKXLVXPYZII-MMTMODRTSA-N
beta-Muricholic acid	DKPMWHFRUGMUKF-CRKPLTDNSA-N
beta-Sitosterol	KZJWDPNRJALLNS-VJSFXXLFSA-N
Bilirubin	BPYKTIZUTYGOLE-IFADSCNNSA-N
Biliverdin	QBUVFDKTZJNUPP-BBROENKCSA-N
Bis-(3,4-dimethyldibenzylidenesorbitol)	YWEWWNPYDDHZDI-JJKKTNRVSA-N
CAY10683	HTOYBIILVCHURC-UHFFFAOYSA-N
Chenodeoxycholic acid	RUDATBOHQWOJDD-BSWAIDMHSA-N
Cholan-24-oic acid, 12-hydroxy-3-oxo-	WMUMZOAFCDOTRW-UHFFFAOYSA-N
Cholan-24-oic acid, 12-hydroxy-3-oxo-, methyl ester	LOJPGRHPJBGMMF-JJNSWQHQSA-N
Cholestan-3-ol, (3 alpha,5 beta)-	QYIXCDOBOSTCEI-VZNZRSCWSA-N
Cholestan-3-one, (5 alpha)-	PESKGJQREUXSRR-UXIWKSIVSA-N
Cholesterol	HVYWMOMLDIMFJA-DPAQBDIFSA-N
Cholesterol 3-sulfate	BHYOQNUELFTYRT-DPAQBDIFSA-N
cis,cis-9,12-Octadecadien-1-ol	JXNPEDYJTDQORS-HZJYTTRNSA-N
cis-10-Nonadecenoic acid	BBOWBNGUEWHNQZ-KTKRTIGZSA-N
cis-13-Eicosenoic acid	URXZXNYJPAJJOQ-FPLPWBNLSA-N
cis-Vaccenic acid	UWHZIFQPPBDJPM-FPLPWBNLSA-N
Citrulline	RHGKLRLOHDJJDR-UHFFFAOYSA-N
Cocamidopropyl betaine	MRUAUOIMASANKQ-UHFFFAOYSA-N
Crotonic acid	LDHQCZJRKDOVOX-NSCUHMNNSA-N
Decaethylene glycol	DTPCFIHYWYONMD-UHFFFAOYSA-N
Dehydropipernonaline	KAYVDASZRFLFRZ-PQECNABGSA-N
Deoxycholic acid	KXGVEGMKQFWNSR-LLQZFEROSA-N
D-erythro-Sphinganine	OTKJDMGTUTTYMP-ZWKOTPCHSA-N
D-Glucosyl-beta-1,1-N-palmitoyl-D-erythro-sphingosine	VJLLLMIZEJJZTE-NNTBDIJYSA-N
Didecyldimethylammonium	JGFDZZLUDWMUQH-UHFFFAOYSA-N
Dihomo-gamma-linolenic acid methyl ester	QHATYOWJCAQINT-JPFHKJGASA-N
Dimethyl azelate	DRUKNYVQGHETPO-UHFFFAOYSA-N
DL-beta-Hydroxypalmitic acid	CBWALJHXHCJYTE-UHFFFAOYSA-N
DL-Indole-3-lactic acid	XGILAAMKEQUXLS-UHFFFAOYSA-N
DL-Serine, succinate (ester)	ZAHSBRLHJRVFAU-UHFFFAOYSA-N
D-Mannosamine	FZHXIRIBWMQPQF-KVTDHHQDSA-N
Dodecanedioic acid	TVIDDXQYHWJXFK-UHFFFAOYSA-N
D-Sphingosine	WWUZIQQURGPMPG-KRWOKUGFSA-N

Table 4. Non-Certified Metabolite Identifications of Omnivore Stool by LC-MS/MS	
Metabolite ID	InChiKey
Enalapril	GBXSMTUPTTWBMN-XIRDDKMYSA-N
Enalaprilat	LZFZMUMEGBBDTC-QEJZJMRPSA-N
Epilupeol	MQYXUWHLBZFQQO-ISZJTHHZSA-N
Ergocalciferol	MECHNRXZTMCUDQ-ANGGWTPUSA-N
Erioglaucine	CTRXDTYTAAKVSM-UHFFFAOYSA-N
Erucamide	UAUDZVJPLUQNMU-KTKRTIGZSA-N
Erythrodiol	PSZDOEIIIJFCFE-KWVOMAKGSA-N
Ethanesulfonic acid, 2-[(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)amino]-	IZRUXXTXKZAGQQ-UHFFFAOYSA-N
Fucosterol	OSELKOCHBMDKEJ-JUGJNGJRSA-N
Geranyllinalool	IQDXAJNQKSIPGB-HQSZAHFGSA-N
Ginkgolic acid I	YXHVCZZLWZYHSA-FPLPWBNLSA-N
Glu-Ile	SNFUTDLOCQQRQD-LKEWCRSYSA-N
Glycerol monooleate	RZRNAYUHWVFMIP-KTKRTIGZSA-N
Glycerol trilaurate	VMPHSYLJUKZBJJ-UHFFFAOYSA-N
Glycodeoxycholic acid	WVULKSPCQVQLCU-UHFFFAOYSA-N
Glycyl-L-norleucine	XVUIZOUTLADVIH-UHFFFAOYSA-N
Gly-Val	STKYPAFSDFAEPH-LURJTMIESA-N
Guanine	UYTPUPDQBNUYGX-UHFFFAOYSA-N
Heptadecasphinganine	KFQUQCFJDMSIJF-DLBZAZTESA-N
Ile-Glu	KTGFOCFYOZQVRJ-ACLDMZEESA-N
Ile-Phe	WMDZARSFSMZOQO-UHTWSYAYSA-N
Ile-Ser	TWVKGYNQQAUNRN-ACZMJKKPSA-N
Ile-Thr	DRCKHKZYDLJYFQ-YWIQKCBGSA-N
Ile-Val	BCXBIONYYJCSDF-CIUDSAMLSA-N
Isobutyric acid	KQNPFQTWMSNSAP-UHFFFAOYSA-N
Kaurane-17,18-dioic acid, 18-methyl ester, (4 alpha,16 alpha)-	YDAVVXOXSSFVPF-BBBHLOGDSA-N
Lactosyl-Ceramide(d18:1/22:0)	QYWVASPEUXEHSY-DYGYHFHFSA-N
Laurylsulfuric acid	MOTZDAYCYVMXPC-UHFFFAOYSA-N
Linoleic Acid	OYHQOLUKZRVURQ-HZJYTTRNSA-N
Linoleic acid-biotin	TXYWCIYPXRNWJU-MJDXKYDGSA-N
Lithocholic acid	SMEROWZSTRWXGI-HVATVPOCSA-N
Lithocholylglycine	XBSQTYHEGZTYJE-OETIFKLTSA-N
Lupeol	MQYXUWHLBZFQQO-QGTGJCAVSA-N
Methionine sulfoxide	QEFRNWWLZKMPFJ-YGVKFDHGSA-N
Methyl deoxycholate	ZHUOOEGSSFNTNP-JMKDMENQSA-N
Methyl hydrogen azelate	VVWPSAPZUZXYCM-UHFFFAOYSA-N
Methyl linolenate	DVWSXZIHSUZZKJ-YSTUJMKBSA-N
Myristyl sulfate	URLJMZWTXZTZRR-UHFFFAOYSA-N
N-(14-Methylpentadecanoyl)phenylalanine	WICAPTTWPBEVPW-UHFFFAOYSA-N
N-(6-Methyl-2-oxohexahydro-4-pyrimidinyl)urea	CZAUMIGWDFREBR-UHFFFAOYSA-N
N-(Octadecanoyl)sphing-4-enine-1-phosphocholine	LKQLRGMMMAHREN-NWBJSICCSA-N
N,N-Dimethylsphingosine	YRXOQXUDKDCXME-YIVRLKKSSA-N
N2-Isobutyryl-2'-deoxyguanosine	SIDXEQFMTMICKG-UHFFFAOYSA-N
N6-Palmitoyl-L-lysine	IWKZTTDNVPAHNP-FQEVSTJZSA-N
N-Acetyl-.beta.-D-mannosamine	OVRNDRQMDRJTHS-OZRXBMAMSA-N

Table 4. Non-Certified Metabolite Identifications of Omnivore Stool by LC-MS/MS	
Metabolite ID	InChiKey
N-Acetyldihydrosphingosine	CRJGESKKUOMBCT-VQTJNVASSA-N
N-Acetyl-D-norleucine	JDMCEGLQFSOMQH-SSDOTTSWSA-N
N-Acetyl-L-glutamine	KSMRODHGGIIXDV-YFKPBYRVSA-N
N-Acetyl-L-glutamic acid	RFMMMVDNIPUKGG-YFKPBYRVSA-N
N-alpha-Acetyl-L-lysine	VEYYWZRYIYDQJM-ZETCQYMHSA-N
N-Benzyl-N,N-dimethyl-1-tetradecanaminium cation	WNBGYVXHFTYOBY-UHFFFAOYSA-N
N-Docosanoyl-4-sphingenyl-1-O-phosphorylcholine	FJJANLYCZUNFSE-TWKUQIQBSA-N
N-epsilon-Acetyl-L-lysine	DTERQYGMUDWYAZ-ZETCQYMHSA-N
Nervonoyl ethanolamide	LISKWSFNVJTQKH-KTKRTIGZSA-N
N-Hexadecyl sulfate	LPTIRUACFKQDHZ-UHFFFAOYSA-N
N-Hexanoylsphingosine	NPRJSFWNFTXXQC-QFWQFVLDSA-N
Nitrobenzene	LQNUZADURLCDLV-UHFFFAOYSA-N
N-Lauroyl-D-erythro-sphinganine	UHWYQXNZIBLESO-URLMMPGGSA-N
N-L-gamma-Glutamyl-L-leucine	MYFMARDICOWMQP-UHFFFAOYSA-N
N-Methyl-L-phenylalanine	SCIFESDRCALIIM-VIFPVBQESA-N
N-Myristoylsphinganine	UDTSZXVRDXQARY-IOWSJCHKSA-N
N-Nervonoyl-D-erythro-sphingosylphosphorylcholine	WKZHECFHXLTOLJ-QYKFWSDSSA-N
N-Octanoylsphingosine	APDLCSPGWPLYEQ-WRBRXSDHSA-N
N-Oleoyl-4-sphingenine	OBFSLMQLPNKVRW-RHPAUOISSA-N
N-Oleoyl-D-erythro-sphinganine	MJQIARGPQMNBGT-WWUCIAQXSA-N
N-Oleoylethanolamine	BOWVQLFMWHZBEF-KTKRTIGZSA-N
Nonaethylene glycol	YZUUTMGDONTGTN-UHFFFAOYSA-N
Nonanedioic acid	BDJRBEYXGGNYIS-UHFFFAOYSA-N
N-Palmitoyl-D-sphingosine	YDNKGFDKKRUKPY-TURZORIXSA-N
N-Stearoylsphinganine	KZTJQXAANJHSCE-OIDHKYIRSA-N
N-Tetracosenoyl-4-sphingenine	VJSBNBBOSZJDKB-KPEYJIHVSA-N
Octaethylene glycol	GLZWNFNQMJAZGY-UHFFFAOYSA-N
Oleamide	FATBGEAMYMYZAF-KTKRTIGZSA-N
Oleoyl ethylamide	JZJYYCFYGXPUMF-QXMHVHEDSA-N
Oleoylserotonin	LCQKHZYXPCLVBI-KTKRTIGZSA-N
Palmitoyl sphingomyelin	RWKUXQNLWDTSLO-GWQJGLRPSA-N
Palmitoyleicosapentaenoyl phosphatidylcholine	KLTHQSWIRFFBRI-KOQZQRJKSA-N
Palmitoyl-L-carnitine	XOMRRQXKHMYMOC-OAQYLSRUSA-N
Pantothenic acid	GHOKWGTUZJEAQD-UHFFFAOYSA-N
PEG Monooleate n8	RRMPJCDMVAUQGF-MDZDMXLPSA-N
PEG14	AKWFJQNBHYVIPY-UHFFFAOYSA-N
PEG16	OWTQQPNDSWCHOV-UHFFFAOYSA-N
Pheophorbide a	NSFSLUUZQIAOOX-QEWKCGBTSA-N
Phe-Val	IEHDJWSAXBGJIP-RYUDHWBXSA-N
Piperchabamide B	CHOLQJRIMZGPNC-QHKWOANTSA-N
Pipernonaline	PKLGRWSJBLGIBF-JMQWPVDRSA-N
Piperolein A	MIWPBXQTBYPJEF-XBXARRHUSA-N
Poly THF n8	RPGZMBUUQBRFFX-UHFFFAOYSA-N
Pregnenolone sulfate	DIJBBUIOWGGQOP-QGVNFLHTSA-N
Prostaglandin K2	LGMXPVXJSFPPTQ-DJUJBXLVSA-N

Table 4. Non-Certified Metabolite Identifications of Omnivore Stool by LC-MS/MS	
Metabolite ID	InChiKey
Pyridoxine	LXNHXLLTXMVWPM-UHFFFAOYSA-N
Pyruvic acid	LCTONWCANYUPML-UHFFFAOYSA-N
Retrofractramide A	BPSWISYORIWKCT-FCGWLDPVSA-N
Riboflavin	AUNGANRZJHBGPY-SCRDCRAPSA-N
Sarsasapogenin	GMBQZIIUCVWOCD-WWASVFFGSA-N
Sebacic acid	CXMXRPHRNRROMY-UHFFFAOYSA-N
Stearamide	LYRFLYHAGKPMFH-UHFFFAOYSA-N
Stearic Acid	QIQXTHQIDYTFRH-UHFFFAOYSA-N
Stearoyl ethanolamide	OTGQIQQTPXJQRG-UHFFFAOYSA-N
Suberic acid	TYFQFVWCELRYAO-UHFFFAOYSA-N
Sucralose	BAQAVOSOZGMPRM-QBMZZYIRSA-N
Sucrose	CZMRCDWAGMRECN-UGDNZRGBSA-N
Tacrolimus	QJJXYPPXXYFBGM-LJIGMGMYSA-N
Tauroursodeoxycholic acid	BHTRKEVKTKCXOH-OGTVOWCVSA-N
Termitomycamide E	JTSNNDBVDQFVEG-HZJYTTRNSA-N
Testosterone sulfate	WAQBISPOEAOCOG-DYKIIFRCSA-N
Tetradecanedioic acid, 5,6-dihydroxy-	JCOCIXAHAFALHI-UHFFFAOYSA-N
Tetrahydroharman-3-carboxylic acid	ZUPHXNBLQCSEIA-UHFFFAOYSA-N
Thiamine cation	JZRWCGZRTZMZEH-UHFFFAOYSA-N
Threonine	AYFVYJQAPQTCCC-UHFFFAOYSA-N
Thr-Glu	BECPPKYKPSRKCP-JCGDXUMPSA-N
Thr-Leu	BQBCIBCLXBKYHW-BIIVOSGPSA-N
Tildipirosin	HNDXPZPJZGTJLJ-UEJFNEDBSA-N
Tomatidine	XYNPYHXGMWJBLV-KLPIGKMYSA-N
trans-Petroselinic acid	CNVZJPUDSLNTQU-OUKQBFOZSA-N
trans-Vaccenic acid	UWHZIFQPPBDJPM-BQYQJAHWSA-N
Tridemorph	YTOPFCCWCSOHFV-UHFFFAOYSA-N
Triethylene glycol bis(2-ethylhexanoate)	FRQDZJMEHSJOPU-UHFFFAOYSA-N
Trihydroxycholestanoic acid	CNWPIIOQKZNXBB-VCVMUKOKSA-N
Trilinolein	HBOQXIRUPVQLKX-BBWANDEASA-N
Tuberonic acid	RZGFUGXQKMEMOO-BSANDHCLSA-N
Uracil	ISAKRJDGNUQOIC-UHFFFAOYSA-N
Uric acid	LEHOTFFKMJEONL-UHFFFAOYSA-N
Urobilin	KDCCOOGTVSRCHX-UYMYUHGCSA-N
Urocanic acid	LOIYMIARKYCTBW-OWOJBTEDSA-N
Val-Ala	HSRXSKHRSXRCFC-WDSKDSINSA-N
Val-Glu	UPJONISHZRADBH-POYBYMJQSA-N
Val-Ile	PNVLWFYAPWAQMU-DJLDLDEBSA-N
Val-Leu	XCTHZFGSVQBHBW-UHFFFAOYSA-N
Val-Val	KRNYOVHEKOBTEF-UHFFFAOYSA-N
Xanthine	LRFVTYWOQMYALW-UHFFFAOYSA-N
Xanthurenic acid	FBZONXHGGPHHIY-UHFFFAOYSA-N

Table 5. Non-Certified Metabolite Identifications of Vegetarian Stool by LC-MS/MS	
Metabolite	InChiKey
alpha-Tocopherol	GVJHHUAWPYXKBD-IEOSBIPESA-N
(15:3)-Anacardic acid	QUVGEKPNSCFQIR-UTOQUPLUSA-N
(1S,2S,3aR,4S,5S,9R,11R,13aS)-4,9,11-tris(acetyloxy)-3a-hydroxy-2,5,8,8,12-pentamethyl-1H,2H,3H,3aH,4H,5H,8H,9H,10H,11H,13aH-cyclopenta[12]annulen-1-yl benzoate	BRVXVMOWTHQKHC-OTOOIOIQSA-N
(2-{4-[(R)-(4-chlorophenyl)(phenyl)methyl]-1-piperazinyl}ethoxy)acetic acid	ZKLPARSLTMPFCP-OAQYLSRUSA-N
(2E,4E,6E)-11-(1,3-Benzodioxol-5-yl)-N-(2-methylpropyl)undeca-2,4,6-trienamide	ITXVWRWWWSDXOY-HNZFQPFYSA-N
(2S)-2-[(3-Methylbutanoyl)amino]pentanedioic acid	HCVIJONZMYVLAW-ZETCQYMHSA-N
(2S-,cis)-5-Benzyl-3,6-dioxo-2-piperazineacetic acid	VNHJXYUDIBQDDX-UWVGGRQHSA-N
(3-beta)-Allopregnanolone sulfate	MENQCIVHHONJLU-FZCSVUEKSA-N
(3-Oxo-2,3-dihydro-4H-1,4-benzoxazin-4-yl)acetic acid	POGLODLVBYOXAO-UHFFFAOYSA-N
(4-Methylphenyl)oxidanesulfonic acid	WGNAKZGUSRVWRH-UHFFFAOYSA-N
(4S)-4-Amino-5-hydroxypentanoic acid	JPYGFLFUDLRNKX-BYPYZUCNSA-N
(6E,10Z,14E)-6,14-Dimethyl-3-methylidene-2-oxo-3a,4,5,8,9,12,13,15a-octahydrocyclotetradeca[b]furan-10-carboxylic acid	SORYERHBQFTRIK-AMVXUGKJSA-N
(Carboxymethyl)dodecyldimethylammonium cation	DVEKCXOJTLDBFE-UHFFFAOYSA-O
1,1-Dimethyl-2,3,4,9-tetrahydro-1H-beta-carboline-3-carboxylic acid	CWGHZIOJFVTEPN-UHFFFAOYSA-N
1,2-Dihexadecanoyl-3-(9Z-octadecenoyl)-sn-glycerol	YHMDGPZOSGBQRH-YYSBDVFPSA-N
1,2-Dilinoleoyl-sn-glycero-3-phosphocholine	FVXDQWZBHIXIEJ-LNDKUQBDSA-N
1,2-Dimyristoyl-sn-glycerol	JFBCSFJKETUREV-LJAQVGFWSA-N
1,2-Dioctadecanoyl-sn-glycerol	UHUSDOQQWJGJQS-QNGWXLTQSA-N
1,2-dioleoyl-sn-glycero-3-phosphatidylcholine	SNKAWJBJQDLSFF-NVKMUCNASA-N
1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine	MWRBNPKJOOWZPW-NYVOMTAGSA-N
1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine-N,N-dimethyl	XHPZRQBHFOVLEJ-UNUIOPIBSA-N
1,2-Dioleoyl-sn-glycerol	AFSHUZFNMVJNKX-LLWMBOQKSA-N
1,2-Dipentadecanoyl-sn-glycero-3-phosphocholine	LJARBVLDSOWRJT-PSXMRANNSA-N
1,3-Diolein	DRAWQKGUORNASA-CLFAGFIQSA-N
1,7-Dimethyluric acid	NOFNCLGCUJJPKU-UHFFFAOYSA-N
12-Methoxycarnosic acid	QQNSARJGBPMQDI-MZVUKIKXSA-N
13-cis-Retinol	FPIPGXGPPPQFEQ-HWCYFHEPSA-N
18-beta-Glycyrrhetinic acid	MPDGHEJMBKOTSU-YKLVYJNSSA-N
1-Arachidoyl-2-hydroxy-sn-glycero-3-phosphocholine	UATOAILWGVYRQS-HHHXNRCGSA-N
1H-Indole-3-propanoic acid	GOLXRNDWAUTYKT-UHFFFAOYSA-N
1-Methyl-3,6-(1H,2H)-pyridazinedione	UAECOHJYXUJDOF-UHFFFAOYSA-N
1-Methyluric acid	QFDRTQONISXGJA-UHFFFAOYSA-N
1-Monolinolenin	GGJRAQULURVTAJ-PDBXOOCHSA-N
1-Octadecanoyl-2-octadecenoyl-sn-glycero-3-phosphocholine	ATHVAWFAEPLPPQ-QPOMNCEOSA-N
1-O-Hexadecyl-2-O-acetyl-sn-glyceryl-3-phosphorylcholine	HVAUUPRFYPCOCA-AREMUKBSSA-N
1-Oleoyl-2-linoleoyl-rac-glycerol	BLZVZPYMHLXLHG-RQOIEFAZSA-N
1-Oleoyl-2-palmitoyl-rac-glycerol	DOZKMFVMCATMEH-ZCXUNETKSA-N
1-Oleoyl-sn-glycero-3-phosphoethanolamine	PYVRVRFVLRNJLY-MZMPXXGTSA-N
1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine	IESVDEZGAHUQJU-ZLBXKVHBSA-N
1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	YVYMBNSKXOXSKW-HXUWFJFHSA-N
1-Palmitoyl-2-linoleoyl-rac-glycerol	SVXWJFFKLMLOHO-BCTRXSSUSA-N
1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine	JLPULHDHAOZNQI-ZTIMHPMXSA-N
1-Palmitoyl-2-oleoyl-3-linoleoyl-rac-glycerol	KGLAHZTWGPHKFF-FBSASISJSA-N

Table 5. Non-Certified Metabolite Identifications of Vegetarian Stool by LC-MS/MS	
Metabolite	InChiKey
1-Palmitoyl-2-oleoyl-sn-glycerol	YEJYLHKQOBOSCP-OZKTZCCCSA-N
1-Palmitoyl-sn-glycero-3-phosphocholine	ASWBNKHCZGQVJV-HSZRJFAPSA-N
1-Pentadecanoyl-sn-glycero-3-phosphocholine	RJZVWDTYEWCUAR-JOCHJYFZSA-N
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine	IHNKQIMGVNPMTC-RUZDIDTESA-N
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	BBYWOYAFBUOUFP-JOCHJYFZSA-N
1-Stearoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine	YDTWOEYVDRKKCR-KNERPIHHSA-N
1-Stearoyl-2-oleoyl-sn-glycero-3-phosphocholine	ATHVAWFAEPLPPQ-VRDBWYNSSA-N
2-({[3-Methyl-4-(2,2,2-trifluoroethoxy)-2-pyridinyl]methyl}sulfanyl)-1H-benzimidazole	CCHLMSUZHFPSFC-UHFFFAOYSA-N
2'-(4-Methylumbelliferyl)-.alpha.-D-N-acetylneuraminic acid	KKDWIUJBUSOPGC-GKHMPSLRSA-N
2-(Hexadecylamino)ethanol	SIFHZKKXWMJWOB-UHFFFAOYSA-N
2-(O-beta-D-Glucopyranosyl)atractyligenin	ZUDBDCBPZHGAEL-ICRASABDSA-N
2,3,4,9-Tetrahydro-1H-beta-carboline-3-carboxylic acid	FSNCEEGOMTYXKY-UHFFFAOYSA-N
2,3-Dihydroxypropyl octadecanoate	VBICKXHEKHSIBG-UHFFFAOYSA-N
2,4-Bis(1,1-dimethylethyl)phenol phosphate	GUDSEWUOWPVZPC-UHFFFAOYSA-N
2-[(2R,4aS,8S,8aS)-8-{2-[(4aS,7R,8aR)-7-(1-Carboxyvinyl)-1-hydroxy-4a-methyl-2-oxo-1,2,4a,5,6,7,8,8a-octahydro-1-naphthalenyl]ethyl}-4a-methyl-7-oxo-1,2,3,4,4a,7,8,8a-octahydro-2-naphthalenyl]acrylic acid	BSSWIRVAMSGQMG-RTTXQYISSA-N
2-[3-[3-Hydroxy-4-(4-hydroxyphenyl)-2,5-dimethoxyphenyl]-5-oxo-2H-furan-2-yl]acetic acid	CLNCCYGZTAZYLJ-UHFFFAOYSA-N
24,25-Epoxylanost-7-ene-3,23-diol	UMTABACRBSGXGK-UHFFFAOYSA-N
2'-Deoxyadenosine	OLXZPDWKRNYJJZ-RRKCRQDMSA-N
2'-Deoxyinosine	VGONTNSXDCQUGY-JXBXZBNISA-N
2-Hydroxypalmitic acid	JGHSBPIZNUXPLA-UHFFFAOYSA-N
2-Linoleoyl-1-palmitoyl-sn-glycero-3-phosphoethanolamine	HBZNVZIRJWODIB-NHCUFCNUSA-N
2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine	WTJKGGKOPKCXLL-VYOBOKEXSA-N
2-Palmitoyl-rac-glycerol	BBNYCLAREVXOSG-UHFFFAOYSA-N
2-Thio-acetyl MAGE	SJNRNWWBXZOALQ-OAQYLSRUSA-N
3-(1H-Imidazol-4-yl)propanoic acid	ZCKYOWGFRHAZIQ-UHFFFAOYSA-N
3-(3-Hydroxyphenyl)-2-oxopropanoic acid	PNYWALDMLUDDTA-UHFFFAOYSA-N
3-(Tetradecylamino)-1-propanol	FDZNQCUTOMWCJE-UHFFFAOYSA-N
3,7,12-Trihydroxycholan-24-oic acid (stereoisomer unknown)	BHQCQFFYRZLCQQ-UHFFFAOYSA-N
3,7-Dimethyluric acid	HMLZLHKHNBLLJD-UHFFFAOYSA-N
3,7-Dimethyluric acid	HMLZLHKHNBLLJD-UHFFFAOYSA-N
3-[5-(2-Methylpropyl)-3,6-dioxopiperazin-2-yl]propanoic acid	CSRXCVLPMJBQIM-UHFFFAOYSA-N
3-Hydroxyurs-12-en-23-oic acid	NBGQZFQREPIKMG-UHFFFAOYSA-N
3-Methylxanthine	GMSNIKWWOQHZGF-UHFFFAOYSA-N
4-(3,4-Dihydroxyphenyl)-6,7-dihydroxy-2-naphthalenecarboxylic acid	ZSKDVJYWOHBGNI-UHFFFAOYSA-N
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	JBAVAJIXZVRJHT-UHFFFAOYSA-N
4-Cholestenone	NYOXRYYXRWJDKP-GYKMGIIDSA-N
4-Ketopimelic acid	UDDSEESQRGPVIL-UHFFFAOYSA-N
4-Oxododecanedioic acid	HHXMOTDTSDYYEI-UHFFFAOYSA-N
4-Pyridoxic acid	HXACOUQIXZGNBF-UHFFFAOYSA-N
5,6-Dihydrouridine	ZPTBLXKRQACLCR-XVFCMESISA-N
5-Hydroxyindole-3-acetic acid	DUUGKQCEGZLZNO-UHFFFAOYSA-N
6-Heptadecen-16-yne-1,2,4-triol	YPRUUOUDKJWVMW-VAWYXSNFSA-N
6-Methyl-1,2,3-oxathiazin-4(3H)-one 2,2-dioxide	YGCFIWIQZPHFLU-UHFFFAOYSA-N

Table 5. Non-Certified Metabolite Identifications of Vegetarian Stool by LC-MS/MS	
Metabolite	InChiKey
8-(3-Octyl-2-oxiranyl)octanoic acid	IMYZYCNQZDBZBQ-UHFFFAOYSA-N
8-Acetamido-2-methyl-7-oxononanoic acid	UALLEVOGEQZKSX-UHFFFAOYSA-N
9,10-Dihydroxy-12Z-octadecenoic acid	XEBKSQSGNGRGDW-CJWPDFJNSA-N
9-Oxo-10(E),12(E)-octadecadienoic acid	LUZSWWYKKLTDHU-SIGMCMEVSA-N
9Z,11E,13E-Octadecatrienoic acid	CUXYLFPMQMFGPL-WPOADVJFSA-N
Adipic acid	WNLRTRBMVRJNCN-UHFFFAOYSA-N
Allyl 4-amino-1-piperidinecarboxylate	XKLGRJGBMKOQDK-UHFFFAOYSA-N
alpha,alpha-Dilaurin	KUVAEMGNHJQSMH-UHFFFAOYSA-N
alpha-Hyodeoxycholic acid methyl ester	BWDRDVHYVJQWBO-QWXHOCAMSA-N
alpha-Tocopheryl acetate	ZAKOWWREFLAJOT-PDNQPUDYSA-N
Anacardic acid	ADFWQBGTDJIESE-UHFFFAOYSA-N
Anacardic acid diene	KAOMOVYHGLSFHQ-UTOQUPLUSA-N
Asn-Pro	GADKFYNESXNRLC-WDSKDSINSA-N
Asp-Pro	UKGGPJNBONZZCM-WDSKDSINSA-N
Asp-Val	CPMKYMGGYUFOHS-CAHLUQPWSA-N
Azaspiracid-8	VTXJIDBQMAXDIY-CQQSUDGLSA-N
Bacilysocin	DIGHTWUQPWHBPG-UHFFFAOYSA-N
Benzenesulfonic acid, 4-(acetylamino)-	ZQPVMSLLKQTRMG-UHFFFAOYSA-N
Benzyldimethyldodecylammonium cation	CYDRXTMLKJDRQH-UHFFFAOYSA-N
Benzyldimethylstearylammonium cation	FWLORMQUOWCQPO-UHFFFAOYSA-N
beta-Cryptoxanthin	DMASLKHVQRHNES-FKKUPVFPSA-N
beta-Hyodeoxycholic acid	DGABKXLVXPYZII-MMTMODRTSA-N
beta-Sitosterol	KZJWDPNRJALLNS-VJSFXXLFSA-N
Bilirubin	BPYKTIZUTYGOLE-IFADSCNNSA-N
Bis-(3,4-dimethyldibenzylidenesorbitol)	YWEWWNPYDDHZDI-JJKKTNRVSA-N
Chenodeoxycholic acid	RUDATBOHQWOJDD-BSWAIDMHSA-N
Cholan-24-oic acid, 12-hydroxy-3-oxo-	WMUMZOAFCDOTRW-UHFFFAOYSA-N
Cholan-24-oic acid, 12-hydroxy-3-oxo-, methyl ester	LOJPGRHPJBGMMF-JJNSWQHQSA-N
Cholestan-3-ol, (3 alpha,5 beta)-	QYIXCDOBOSTCEI-VZNZRSCWSA-N
Cholesterol	HVYWMOMLDIMFJA-DPAQBDIFSA-N
Cholesterol 3-sulfate	BHYOQNUELFTYRT-DPAQBDIFSA-N
Cholic acid	BHQCQFFYRZLCQQ-OELDTZBJSA-N
cis,cis-9,12-Octadecadien-1-ol	JXNPEDYJTDQORS-HZJYTTRNSA-N
cis-Vaccenic acid	UWHZIFQPPBDJPM-FPLPWBNLSA-N
Citrulline	RHGKLRLOHDJJDR-UHFFFAOYSA-N
Cocamidopropyl betaine	MRUAUOIMASANKQ-UHFFFAOYSA-N
D-alpha-Tocopherol succinate	IELOKBJPULMYRW-NJQVLOCASA-N
Dehydropipernonaline	KAYVDASZRFLFRZ-PQECNABGSA-N
Deoxycholic acid	KXGVEGMKQFWNSR-LLQZFEROSA-N
D-erythro-N-Stearoylsphingosine	WWUZIQQURGPMPG-KRWOKUGFSA-N
D-erythro-Sphinganine	OTKJDMGTUTTYMP-ZWKOTPCHSA-N
D-Glucosyl-beta-1,1-N-palmitoyl-D-erythro-sphingosine	VJLLLMIZEJJZTE-NNTBDIJYSA-N
Didymin	RMCRQBAILCLJGU-HIBKWJPLSA-N
Dihydrodaidzein	JHYXBPPMXZIHKG-UHFFFAOYSA-N
Dimethyl azelate	DRUKNYVQGHETPO-UHFFFAOYSA-N

Table 5. Non-Certified Metabolite Identifications of Vegetarian Stool by LC-MS/MS	
Metabolite	InChiKey
Di-tert-butyl L-glutamate	NTUGPDFKMVHCCJ-VIFPVBQESA-N
DL-beta-Hydroxypalmitic acid	CBWALJHXHCJYTE-UHFFFAOYSA-N
DL-Indole-3-lactic acid	XGILAAMKEQUXLS-UHFFFAOYSA-N
DL-Serine, succinate (ester)	ZAHSBRLHJRVFAU-UHFFFAOYSA-N
Docosanoyl ethanolamide	XHFWUECSNJWBJU-UHFFFAOYSA-N
Dodecanedioic acid	TVIDDXQYHWJXFK-UHFFFAOYSA-N
Ergocalciferol	MECHNRXZTMCUDQ-ANGGWTPUSA-N
Erucamide	UAUDZVJPLUQNMU-KTKRTIGZSA-N
Formamide, N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-N-[4-hydroxy-1-methyl-2-(propyldithio)-1-buten-1-yl]-	UDCIYVVYDCXLSX-SDNWHVSQSA-N
Gabapentin	UGJMXCAKCUNAIE-UHFFFAOYSA-N
Gamithromycin	VWAMTBXLZPEDQO-UZSBJOJWSA-N
gamma-Glu-Phe	XHHOHZPNYFQJKL-QWRGUYRKSA-N
Genkwanin	JPMYFOBNRRGFNO-UHFFFAOYSA-N
Ginkgolic acid I	YXHVCZZLWZYHSA-FPLPWBNLSA-N
Gln-Val	MRVYVEQPNDSWLH-XPUUQOCRSA-N
Glu-Glu	KOSRFJWDECSPRO-UHFFFAOYSA-N
Glu-Leu	YBAFDPFAUTYYRW-SFYZADRCSA-N
Glycerol monooleate	RZRNAYUHWVFMIP-KTKRTIGZSA-N
Glycerol trilaurate	VMPHSYLJUKZBJJ-UHFFFAOYSA-N
Glycerol trioleate	PHYFQTYBJUILEZ-IUPFWZBJSA-N
Glycodeoxycholic acid	WVULKSPCQVQLCU-UHFFFAOYSA-N
Gly-Pro	KZNQNBZMBZJQJO-YFKPBYRVSA-N
Gly-Val	STKYPAFSDFAEPH-LURJTMIESA-N
Guanine	UYTPUPDQBNUYGX-UHFFFAOYSA-N
Guanosine	NYHBQMYGNKIUIF-UUOKFMHZSA-N
Guanosine 3',5'-cyclic monophosphate	ZOOGRGPOEVQQDX-BDXYJKHTSA-N
Guineensine	FPMPOFBEYSSYDQ-AUVZEZIHSA-N
Heptadecasphinganine	KFQUQCFJDMSIJF-DLBZAZTESA-N
His-Pro	LNCFUHAPNTYMJB-IUCAKERBSA-N
Histidine	HNDVDQJCIGZPNO-UHFFFAOYSA-N
Ile-Glu	KTGFOCFYOZQVRJ-ACLDMZEESA-N
Ile-Phe	WMDZARSFSMZOQO-UHTWSYAYSA-N
Ile-Thr	DRCKHKZYDLJYFQ-YWIQKCBGSA-N
Ile-Val	BCXBIONYYJCSDF-CIUDSAMLSA-N
Inositol hexanicotinate	MFZCIDXOLLEMOO-GYSGTQPESA-N
Lactosyl-Ceramide(d18:1/22:0)	QYWVASPEUXEHSY-DYGYHFHFSA-N
Laurylsulfuric acid	MOTZDAYCYVMXPC-UHFFFAOYSA-N
Leu-Leu	LCPYQJIKPJDLLB-ZJUUUORDSA-N
Leu-Pro	VTJUNIYRYIAIHF-IUCAKERBSA-N
Linoleic acid-biotin	TXYWCIYPXRNWJU-MJDXKYDGSA-N
Linoleoyl ethanolamide	KQXDGUVSAAQARU-HZJYTTRNSA-N
Lithocholic acid	SMEROWZSTRWXGI-HVATVPOCSA-N
Lumichrome	ZJTJUVIJVLLGSP-UHFFFAOYSA-N
Lysine	KDXKERNSBIXSRK-UHFFFAOYSA-N
Lys-Leu	ATIPDCIQTUXABX-UWVGGRQHSA-N

Table 5. Non-Certified Metabolite Identifications of Vegetarian Stool by LC-MS/MS	
Metabolite	InChiKey
Lys-Pro	AIXUQKMMBQJZCU-IUCAKERBSA-N
Methionine sulfoxide	QEFRNWWLZKMPFJ-YGVKFDHGSA-N
Methyl linolenate	DVWSXZIHSUZZKJ-YSTUJMKBSA-N
Met-Pro	DZMGFGQBRYWJOR-YUMQZZPRSA-N
Met-Val	BJFJQOMZCSHBMY-SFYZADRCSA-N
Monobehenin	OKMWKBLSFKFYGZ-UHFFFAOYSA-N
Myristyl sulfate	URLJMZWTXZTZRR-UHFFFAOYSA-N
N-(14-Methylpentadecanoyl)phenylalanine	WICAPTTWPBEVPW-UHFFFAOYSA-N
N-(2-Amino-4-methylpentanoyl)phenylalanine	KFKWRHQBZQICHA-UHFFFAOYSA-N
N,N-Dimethylsphingosine	YRXOQXUDKDCXME-YIVRLKKSSA-N
N2-Isobutyryl-2'-deoxyguanosine	SIDXEQFMTMICKG-UHFFFAOYSA-N
N6-Palmitoyl-L-lysine	IWKZTTDNVPAHNP-FQEVSTJZSA-N
N-Acetyldihydrosphingosine	CRJGESKKUOMBCT-VQTJNVASSA-N
N-Acetyl-L-alanine	KTHDTJVBEPMMGL-UHFFFAOYSA-N
N-Acetyl-L-aspartic acid	OTCCIMWXFLJLIA-BYPYZUCNSA-N
N-Acetyl-L-glutamic acid	RFMMMVDNIPUKGG-YFKPBYRVSA-N
N-Acetyl-L-tyrosine	CAHKINHBCWCHCF-JTQLQIEISA-N
N-Acetylputrescine	KLZGKIDSEJWEDW-UHFFFAOYSA-N
N-Acetyltyramine	ATDWJOOPFDQZNK-UHFFFAOYSA-N
Nadolol	VWPOSFSPZNDTMJ-UCWKZMIHSA-N
N-alpha-Acetyl-L-lysine	VEYYWZRYIYDQJM-ZETCQYMHSA-N
N-Benzyl-N,N-dimethyl-1-tetradecanaminium cation	WNBGYVXHFTYOBY-UHFFFAOYSA-N
N-Desmethylloperamide	ZMOPTLXEYOVARP-UHFFFAOYSA-N
N-Docosanoyl-4-sphingenyl-1-O-phosphorylcholine	FJJANLYCZUNFSE-TWKUQIQBSA-N
N-Lauroyl-D-erythro-sphinganine	UHWYQXNZIBLESO-URLMMPGGSA-N
N-L-gamma-Glutamyl-L-leucine	MYFMARDICOWMQP-UHFFFAOYSA-N
N-Methyl-L-phenylalanine	SCIFESDRCALIIM-VIFPVBQESA-N
N-Oleoyl-4-sphingenine	OBFSLMQLPNKVRW-RHPAUOISSA-N
N-Oleoyl-D-erythro-sphinganine	MJQIARGPQMNBGT-WWUCIAQXSA-N
N-Palmitoyl-D-sphingosine	YDNKGFDKKRUKPY-TURZORIXSA-N
N-Palmitoyltryptamine	YZWBXGMMZOEBAN-UHFFFAOYSA-N
N-Stearoylsphinganine	KZTJQXAANJHSCE-OIDHKYIRSA-N
N-Tetracosenoyl-4-sphingenine	VJSBNBBOSZJDKB-KPEYJIHVSA-N
Oleanolic acid	MIJYXULNPSFWEK-GTOFXWBISA-N
Oleic acid	ZQPPMHVWECSIRJ-KTKRTIGZSA-N
Oleoyl ethanolamide	BOWVQLFMWHZBEF-KTKRTIGZSA-N
Oleoyl ethylamide	JZJYYCFYGXPUMF-QXMHVHEDSA-N
Oleyl sulfate	ZUBJEHHGZYTRPH-KTKRTIGZSA-N
Palmitoyl ethanolamide	HXYVTAGFYLMHSO-UHFFFAOYSA-N
Palmitoyl sphingomyelin	RWKUXQNLWDTSLO-GWQJGLRPSA-N
Palmitoyleicosapentaenoyl phosphatidylcholine	KLTHQSWIRFFBRI-KOQZQRJKSA-N
Pantothenic acid	GHOKWGTUZJEAQD-UHFFFAOYSA-N
PEG15	ILLKMACMBHTSHP-UHFFFAOYSA-N
PEG16	OWTQQPNDSWCHOV-UHFFFAOYSA-N
Pentacosanoic acid	MWMPEAHGUXCSMY-UHFFFAOYSA-N

Table 5. Non-Certified Metabolite Identifications of Vegetarian Stool by LC-MS/MS	
Metabolite	InChiKey
Pheophorbide a	NSFSLUUZQIAOOX-QEWKCGBTSA-N
Phe-Val	IEHDJWSAXBGJIP-RYUDHWBXSA-N
Phytosphingosine 1-phosphate	AYGOSKULTISFCW-KSZLIROESA-N
Piperine	MXXWOMGUGJBKIW-YPCIICBESA-N
Pregnanetriol	SCPADBBISMMJAW-UHHUKTEYSA-N
Pregnenolone sulfate	DIJBBUIOWGGQOP-QGVNFLHTSA-N
Pro-Val	AWJGUZSYVIVZGP-YUMQZZPRSA-N
Riboflavin	AUNGANRZJHBGPY-SCRDCRAPSA-N
Ricinoleic acid	WBHHMMIMDMUBKC-QJWNTBNXSA-N
Saccharin	CVHZOJJKTDOEJC-UHFFFAOYSA-N
Secalciferol	FCKJYANJHNLEEP-XRWYNYHCSA-N
Ser-Pro	WBAXJMCUFIXCNI-WDSKDSINSA-N
Sertraline	VGKDLMBJGBXTGI-YVEFUNNKSA-N
Stearamide	LYRFLYHAGKPMFH-UHFFFAOYSA-N
Stearoyl ethanolamide	OTGQIQQTPXJQRG-UHFFFAOYSA-N
Stercobilin	TYOWQSLRVAUSMI-WKULSOCRSA-N
Stigmastadienone	MKGZDUKUQPPHFM-DPZQRLQDSA-N
Suberic acid	TYFQFVWCELRYAO-UHFFFAOYSA-N
Sucralose	BAQAVOSOZGMPRM-QBMZZYIRSA-N
Termitomycamide E	JTSNNDBVDQFVEG-HZJYTTRNSA-N
Terrestribisamide	CHEMZHJQHCVLFI-MKICQXMISA-N
Tetradecanedioic acid	HQHCYKULIHKCEB-UHFFFAOYSA-N
Tetradecanedioic acid, 5,6-dihydroxy-	JCOCIXAHAFALHI-UHFFFAOYSA-N
Tetrahydroharman-3-carboxylic acid	ZUPHXNBLQCSEIA-UHFFFAOYSA-N
Thiamine cation	JZRWCGZRTZMZEH-UHFFFAOYSA-N
Threonine	AYFVYJQAPQTCCC-UHFFFAOYSA-N
Thr-Leu	BQBCIBCLXBKYHW-BIIVOSGPSA-N
Thr-Val	CKHWEVXPLJBEOZ-QYNIQEEDSA-N
Tomatidine	XYNPYHXGMWJBLV-KLPIGKMYSA-N
trans-Petroselinic Acid	CNVZJPUDSLNTQU-OUKQBFOZSA-N
trans-Vaccenic acid	UWHZIFQPPBDJPM-BQYQJAHWSA-N
Tridemorph	YTOPFCCWCSOHFV-UHFFFAOYSA-N
Trihydroxycholestanoic acid	CNWPIIOQKZNXBB-VCVMUKOKSA-N
Trilinolein	HBOQXIRUPVQLKX-BBWANDEASA-N
Tyr-Pro	VNYDHJARLHNEGA-RYUDHWBXSA-N
Tyr-Val	OYOQKMOWUDVWCR-RYUDHWBXSA-N
Ubiquinone 9	UUGXJSBPSRROMU-WJNLUYJISA-N
Uracil	ISAKRJDGNUQOIC-UHFFFAOYSA-N
Uric acid	LEHOTFFKMJEONL-UHFFFAOYSA-N
Urobilin	KDCCOOGTVSRCHX-UYMYUHGCSA-N
Urocanic acid	LOIYMIARKYCTBW-OWOJBTEDSA-N
Val-Glu	UPJONISHZRADBH-POYBYMJQSA-N
Val-Pro	GIAZPLMMQOERPN-YUMQZZPRSA-N
Val-Val	KRNYOVHEKOBTEF-UHFFFAOYSA-N
Valylphenylalanine	GJNDXQBALKCYSZ-UHFFFAOYSA-N

Table 5. Non-Certified Metabolite Identifications of Vegetarian Stool by LC-MS/MS	
Metabolite	InChiKey
Victoria Pure Blue BO	ALMMLSQBERCMRB-UHFFFAOYSA-O
Xanthine	LRFVTYWOQMYALW-UHFFFAOYSA-N

Table 6. Non-Certified Metabolite Identifications of Omnivore Stool by NMR	
Metabolite	InChiKey
(3-carboxypropyl)trimethylammonium[(a)]	JHPNVNIEXXLNTR-UHFFFAOYSA-O
1,3-Dihydroxyacetone[(b)]	RXKJFZQQPQGTFL-UHFFFAOYSA-N
1,7-Dimethyluric acid[(a)]	NOFNCLGCUJJPKU-UHFFFAOYSA-N
2-Aminobutyrate[(a)]	QWCKQJZIFLGMSD-UHFFFAOYSA-N
2'-Deoxyuridine[(a)]	MXHRCPNRJAMMIM-UHFFFAOYSA-N
2-Methylbutyrate[(a)]	WLAMNBDJUVNPJU-BYPYZUCNSA-N
3-Hydroxyphenylacetate[(a)]	FVMDYYGIDFPZAX-UHFFFAOYSA-N
3-Methyl-2-oxovalerate[(a)]	JVQYSWDUAOAHFM-UHFFFAOYSA-M
3-Phenylpropionate[(a)(b)]	XMIIGOLPHOKFCH-UHFFFAOYSA-N
4-Hydroxyphenylacetate[(a)]	XQXPVVBIMDBYFF-UHFFFAOYSA-M
4-Hydroxyphenylpropionate[(a)]	ZHMMPVANGNPCBW-UHFFFAOYSA-M
5-Aminopentanoate[(a)]	JJMDCOVWQOJGCB-UHFFFAOYSA-M
Acetate[(a)(b)]	QTBSBXVTEAMEQO-UHFFFAOYSA-M
Alanine[(a)(b)]	QNAYBMKLOCPYGJ-UHFFFAOYSA-N
Alpha-ketoisovaleric acid[(a)]	QHKABHOOEWYVLI-UHFFFAOYSA-N
Aminocaproic acid[(a)]	SLXKOJJOQWFEFD-UHFFFAOYSA-N
Arabinose[(a)(b)]	SRBFZHDQGSBBOR-HWQSCIPKSA-N
Aspartate[(a)(b)]	CKLJMWTZIZZHCS-UHFFFAOYSA-L
Beta-Alanine[(a)]	UCMIRNVEIXFBKS-UHFFFAOYSA-N
Butyrate[(a)(b)]	FERIUCNNQQJTOY-UHFFFAOYSA-M
Cadaverine[(a)(b)]	VHRGRCVQAFMJIZ-UHFFFAOYSA-N
Caprylate[(a)(b)]	WWZKQHOCKIZLMA-UHFFFAOYSA-N
Choline[(a)(b)]	OEYIOHPDSNJKLS-UHFFFAOYSA-N
Citrulline[(a)(b)]	RHGKLRLOHDJJDR-UHFFFAOYSA-N
Deoxycholic acid[(a)]	KXGVEGMKQFWNSR-LLQZFEROSA-N
Desaminotyrosine[(a)(b)]	NMHMNPHRMNGLLB-UHFFFAOYSA-N
Dimethylamine[(b)]	ROSDSFDQCJNGOL-UHFFFAOYSA-N
Ethanolamine[(a)]	HZAXFHJVJLSVMW-UHFFFAOYSA-N
Formate[(a)]	BDAGIHXWWSANSR-UHFFFAOYSA-M
Fructose[(a)]	BJHIKXHVCXFQLS-UHFFFAOYSA-N
Fucose[(a)]	PNNNRSAQSRJVSB-UHFFFAOYSA-N
Fumarate[(a)]	VZCYOOQTPOCHFL-OWOJBTEDSA-L
Galactose[(a)(b)]	GZCGUPFRVQAUEE-UHFFFAOYSA-N
Galacturonic acid[(a)]	IAJILQKETJEXLJ-RSJOWCBRSA-N
Gluconate[(a)]	RGHNJXZEOKUKBD-UHFFFAOYSA-M
Glucose[(a)(b)]	GZCGUPFRVQAUEE-UHFFFAOYSA-N
Glutamate[(a)(b)]	WHUUTDBJXJRKMK-UHFFFAOYSA-N
Glutamine[(a)(b)]	ZDXPYRJPNDTMRX-UHFFFAOYSA-N

Table 6. Non-Certified Metabolite Identifications of Omnivore Stool by NMR	
Metabolite	InChiKey
Glutarate[(a)]	JFCQEDHGNNZCLN-UHFFFAOYSA-N
Glycerol[(a)(b)]	PEDCQBHIVMGVHV-UHFFFAOYSA-N
Glycine[(a)(b)]	DHMQDGOQFOQNFH-UHFFFAOYSA-N
Glycolate[(a)]	AEMRFAOFKBGASW-UHFFFAOYSA-M
Hexanoic acid[(a)]	FUZZWVXGSFPDMH-UHFFFAOYSA-N
Hypoxanthine[(a)(b)]	FDGQSTZJBFJUBT-UHFFFAOYSA-N
Isobutyrate[(a)]	KQNPFQTWMSNSAP-UHFFFAOYSA-M
Isoleucine[(a)(b)]	AGPKZVBTJJNPAG-WHFBIAKZSA-N
Isovalerate[(a)(b)]	GWYFCOCPABKNJV-UHFFFAOYSA-N
Lactate[(a)]	JVTAAEKCZFNVCJ-UHFFFAOYSA-M
Leucine[(a)(b)]	ROHFNLRQFUQHCH-UHFFFAOYSA-N
Lysine[(a)(b)]	KDXKERNSBIXSRK-UHFFFAOYSA-N
Malate[(a)(b)]	BJEPYKJPYRNKOW-UHFFFAOYSA-L
Maltose[(a)]	DKXNBNKWCZZMJT-SILGPGCPSA-N
Mannose[(a)]	GZCGUPFRVQAUEE-UHFFFAOYSA-N
Methanol[(a)(b)]	OKKJLVBELUTLKV-UHFFFAOYSA-N
Methionine[(a)(b)]	FFEARJCKVFRZRR-UHFFFAOYSA-N
Methionine sulfoxide[(a)]	QEFRNWWLZKMPFJ-YGVKFDHGSA-N
Methylamine[(a)]	BAVYZALUXZFZLV-UHFFFAOYSA-N
Methylsuccinate[(a)(b)]	MUXOBHXGJLMRAB-UHFFFAOYSA-N
myo-Inositol[(a)]	CDAISMWEOUEBRE-UHFFFAOYSA-N
N-Acetylalanine[(a)]	KTHDTJVBEPMMGL-VKHMYHEASA-N
N-Acetylglucosamine[(a)]	MBLBDJOUHNCFQT-UHFFFAOYSA-N
N-acetylglutamine[(a)]	KSMRODHGGIIXDV-YFKPBYRVSA-N
Nicotinate[(a)(b)]	PVNIIMVLHYAWGP-UHFFFAOYSA-M
Ornithine[(a)]	AHLPHDHHMVZTML-UHFFFAOYSA-N
Pantothenate[(a)]	GHOKWGTUZJEAQD-UHFFFAOYSA-N
p-Cresol[(b)]	IWDCLRJOBJJRNH-UHFFFAOYSA-N
Phenylacetate[(a)(b)]	IPBVNPXQWQGGJP-UHFFFAOYSA-N
Phenylalanine[(a)(b)]	COLNVLDHVKWLRT-UHFFFAOYSA-N
Pipecolic acid[(a)]	HXEACLLIILLPRG-UHFFFAOYSA-N
Proline[(a)(b)]	ONIBWKKTOPOVIA-UHFFFAOYSA-N
Propionate[(a)(b)]	XBDQKXXYIPTUBI-UHFFFAOYSA-M
Pyroglutamate[(a)]	ODHCTXKNWHHXJC-UHFFFAOYSA-M
Ribose[(a)(b)]	PYMYPHUHKUWMLA-UHFFFAOYSA-N
Serine[(a)(b)]	MTCFGRXMJLQNBG-UHFFFAOYSA-N
Stachydrine[(a)]	CMUNUTVVOOHQPW-UHFFFAOYSA-N
Succinate[(a)(b)]	KDYFGRWQOYBRFD-UHFFFAOYSA-L
Threonine[(a)(b)]	AYFVYJQAPQTCCC-UHFFFAOYSA-N
Thymidine[(a)]	IQFYYKKMVGJFEH-XLPZGREQSA-N
Thymine[(a)]	RWQNBRDOKXIBIV-UHFFFAOYSA-N
Tryptophan[(a)(b)]	QIVBCDIJIAJPQS-UHFFFAOYSA-N
Tyrosine[(a)(b)]	OUYCCCASQSFEME-UHFFFAOYSA-N
Uracil[(a)(b)]	ISAKRJDGNUQOIC-UHFFFAOYSA-N
Uridine[(a)]	DRTQHJPVMGBUCF-XVFCMESISA-N

Table 6. Non-Certified Metabolite Identifications of Omnivore Stool by NMR	
Metabolite	InChiKey
Urocanate[(a)]	LOIYMIARKYCTBW-OWOJBTEDSA-N
Valerate[(a)(b)]	NQPDZGIKBAWPEJ-UHFFFAOYSA-M
Valine[(a)(b)]	KZSNJWFQEVHDMF-UHFFFAOYSA-N
Xanthine[(b)]	LRFVTYWOQMYALW-UHFFFAOYSA-N
Xylose[(b)]	SRBFZHDQGSBBOR-IOVATXLUSA-N

[(a)]Method 1 (Omnivore solvent extraction – polar metabolites)
[(b)]Method 2 (Omnivore aqueous extraction – fecal water)

Table 7. Non-Certified Metabolite Identifications of Vegetarian Stool by NMR	
Metabolite	InChiKey
(3-carboxypropyl)trimethylammonium[(a)]	JHPNVNIEXXLNTR-UHFFFAOYSA-O
1,3-Dimethyluric acid[(a)]	OTSBKHHWSQYEHK-UHFFFAOYSA-N
1-Methyluric acid[(a)]	QFDRTQONISXGJA-UHFFFAOYSA-N
2-Aminobutyrate[(a)]	QWCKQJZIFLGMSD-UHFFFAOYSA-N
2'-Deoxyuridine[(a)]	MXHRCPNRJAMMIM-UHFFFAOYSA-N
2-Methylbutyrate[(a)]	WLAMNBDJUVNPJU-BYPYZUCNSA-N
3-Hydroxyphenylacetate[(a)]	FVMDYYGIDFPZAX-UHFFFAOYSA-N
3-Phenylpropionate[(a)(b)]	XMIIGOLPHOKFCH-UHFFFAOYSA-N
4-Hydroxyphenylacetate[(a)]	XQXPVVBIMDBYFF-UHFFFAOYSA-M
5-Aminopentanoate[(a)]	JJMDCOVWQOJGCB-UHFFFAOYSA-M
6-Hydroxynicotinate[(a)]	BLHCMGRVFXRYRN-UHFFFAOYSA-M
Acetate[(a)(b)]	QTBSBXVTEAMEQO-UHFFFAOYSA-M
Alanine[(a)(b)]	QNAYBMKLOCPYGJ-UHFFFAOYSA-N
Aminocaproic acid[(a)]	SLXKOJJOQWFEFD-UHFFFAOYSA-N
Arabinose[(a)(b)]	SRBFZHDQGSBBOR-HWQSCIPKSA-N
Asparagine[(a)]	DCXYFEDJOCDNAF-REOHCLBHSA-N
Aspartate[(a)(b)]	CKLJMWTZIZZHCS-UHFFFAOYSA-L
Beta-Alanine[(a)]	UCMIRNVEIXFBKS-UHFFFAOYSA-N
Butyrate[(a)(b)]	FERIUCNNQQJTOY-UHFFFAOYSA-M
Cadaverine[(a)(b)]	VHRGRCVQAFMJIZ-UHFFFAOYSA-N
Caprylate[(a)(b)]	WWZKQHOCKIZLMA-UHFFFAOYSA-N
Choline[(a)(b)]	OEYIOHPDSNJKLS-UHFFFAOYSA-N
Citrulline[(a)(b)]	RHGKLRLOHDJJDR-UHFFFAOYSA-N
Deoxycholic acid[(a)]	KXGVEGMKQFWNSR-LLQZFEROSA-N
Ethanolamine[(a)]	HZAXFHJVJLSVMW-UHFFFAOYSA-N
Formate[(a)(b)]	BDAGIHXWWSANSR-UHFFFAOYSA-M
Fructose[(a)]	BJHIKXHVCXFQLS-UHFFFAOYSA-N
Fucose[(a)]	PNNNRSAQSRJVSB-UHFFFAOYSA-N
Fumarate[(a)(b)]	VZCYOOQTPOCHFL-OWOJBTEDSA-L
Gabapentin[(a)(b)]	UGJMXCAKCUNAIE-UHFFFAOYSA-N
Galactose[(a)(b)]	GZCGUPFRVQAUEE-UHFFFAOYSA-N
Galacturonic acid[(a)]	IAJILQKETJEXLJ-RSJOWCBRSA-N
Gluconate[(a)]	RGHNJXZEOKUKBD-UHFFFAOYSA-M
Glucose[(a)(b)]	GZCGUPFRVQAUEE-UHFFFAOYSA-N
Glutamate[(a)(b)]	WHUUTDBJXJRKMK-UHFFFAOYSA-N

Table 7. Non-Certified Metabolite Identifications of Vegetarian Stool by NMR	
Metabolite	InChiKey
Glutamine[(a)(b)]	ZDXPYRJPNDTMRX-UHFFFAOYSA-N
Glycerol[(a)(b)]	PEDCQBHIVMGVHV-UHFFFAOYSA-N
Glycine[(a)(b)]	DHMQDGOQFOQNFH-UHFFFAOYSA-N
Glycolate[(a)]	AEMRFAOFKBGASW-UHFFFAOYSA-M
Hexanoic acid[(a)]	FUZZWVXGSFPDMH-UHFFFAOYSA-N
Hypoxanthine[(a)(b)]	FDGQSTZJBFJUBT-UHFFFAOYSA-N
Isobutyrate[(a)]	KQNPFQTWMSNSAP-UHFFFAOYSA-M
Isoleucine[(a)(b)]	AGPKZVBTJJNPAG-WHFBIAKZSA-N
Isovalerate[(a)(b)]	GWYFCOCPABKNJV-UHFFFAOYSA-N
Lactate[(a)(b)]	JVTAAEKCZFNVCJ-UHFFFAOYSA-M
Leucine[(a)(b)]	ROHFNLRQFUQHCH-UHFFFAOYSA-N
Lysine[(a)(b)]	KDXKERNSBIXSRK-UHFFFAOYSA-N
Malate[(a)(b)]	BJEPYKJPYRNKOW-UHFFFAOYSA-L
Maltose[(a)]	DKXNBNKWCZZMJT-SILGPGCPSA-N
Mannobiose[(a)]	GUBGYTABKSRVRQ-PZPXDAEZSA-N
Methanol[(a)(b)]	OKKJLVBELUTLKV-UHFFFAOYSA-N
Methionine[(a)(b)]	FFEARJCKVFRZRR-UHFFFAOYSA-N
Methionine sulfoxide[(a)]	QEFRNWWLZKMPFJ-YGVKFDHGSA-N
Methylamine[(a)]	BAVYZALUXZFZLV-UHFFFAOYSA-N
Methylsuccinate[(a)(b)]	MUXOBHXGJLMRAB-UHFFFAOYSA-N
myo-Inositol[(a)]	CDAISMWEOUEBRE-UHFFFAOYSA-N
N-Acetylalanine[(a)]	KTHDTJVBEPMMGL-VKHMYHEASA-N
N-Acetylglucosamine[(a)]	MBLBDJOUHNCFQT-UHFFFAOYSA-N
N-acetylglutamine[(a)]	KSMRODHGGIIXDV-YFKPBYRVSA-N
Nicotinate[(a)(b)]	PVNIIMVLHYAWGP-UHFFFAOYSA-M
Ornithine[(a)]	AHLPHDHHMVZTML-UHFFFAOYSA-N
Pantothenate[(a)]	GHOKWGTUZJEAQD-UHFFFAOYSA-N
p-Cresol[(b)]	IWDCLRJOBJJRNH-UHFFFAOYSA-N
Phenylacetate[(a)(b)]	IPBVNPXQWQGGJP-UHFFFAOYSA-N
Phenylalanine[(a)(b)]	COLNVLDHVKWLRT-UHFFFAOYSA-N
Pipecolic acid[(a)]	HXEACLLIILLPRG-UHFFFAOYSA-N
Proline[(a)(b)]	ONIBWKKTOPOVIA-UHFFFAOYSA-N
Propionate[(a)(b)]	XBDQKXXYIPTUBI-UHFFFAOYSA-M
Pyroglutamate[(a)]	ODHCTXKNWHHXJC-UHFFFAOYSA-M
Ribose[(a)(b)]	PYMYPHUHKUWMLA-UHFFFAOYSA-N
Sarcosine[b]	FSYKKLYZXJSNPZ-UHFFFAOYSA-N
Serine[(a)(b)]	MTCFGRXMJLQNBG-UHFFFAOYSA-N
Succinate[(a)(b)]	KDYFGRWQOYBRFD-UHFFFAOYSA-L
Threonine[(a)(b)]	AYFVYJQAPQTCCC-UHFFFAOYSA-N
Thymidine[(a)]	IQFYYKKMVGJFEH-XLPZGREQSA-N
Thymine[(a)]	RWQNBRDOKXIBIV-UHFFFAOYSA-N
Tryptophan[(a)(b)]	QIVBCDIJIAJPQS-UHFFFAOYSA-N
Tyrosine[(a)(b)]	OUYCCCASQSFEME-UHFFFAOYSA-N
Uracil[(a)(b)]	ISAKRJDGNUQOIC-UHFFFAOYSA-N
Uridine[(a)(b)]	DRTQHJPVMGBUCF-XVFCMESISA-N

Table 7. Non-Certified Metabolite Identifications of Vegetarian Stool by NMR	
Metabolite	InChiKey
Urocanate[(a)(b)]	LOIYMIARKYCTBW-OWOJBTEDSA-N
Valerate[(a)(b)]	NQPDZGIKBAWPEJ-UHFFFAOYSA-M
Valine[(a)(b)]	KZSNJWFQEVHDMF-UHFFFAOYSA-N
Xanthine[(b)]	LRFVTYWOQMYALW-UHFFFAOYSA-N
Xylose[(b)]	SRBFZHDQGSBBOR-IOVATXLUSA-N

[(a)]Method 1 (Vegetarian solvent extraction – polar metabolites)
[(b)]Method 2 (Vegetarian aqueous extraction – fecal water)

Safety: RM 8408 IS INTENDED FOR RESEARCH USE ONLY. This is a human source material (human feces). RM 8408 is a Biosafety Level 2 material and should be handled according to applicable federal, state, and/or local regulations and according to policies and procedures of recipient's organization. The supplier has reported that each donor of stool used in the preparation of this product was tested by FDA-licensed tests and found to be negative for human immunodeficiency virus (HIV), HIV-1 antigen, hepatitis B surface antigen, and hepatitis C.

Storage: The original unopened vials of RM 8048 should be stored at −80 °C. Each vial is meant to be a single use. Freeze-thaw cycles of the materials should be avoided.

Usage and Privacy Agreement: NIST does not possess any identifiable private information or any code to identify any identifiable private information related to the Material and will not provide the Purchaser with any identifiable private information of any living individual or any code to identify any identifiable private information related to the Material. Purchaser agrees not to attempt to decipher any identifiable private information from the Material or to identify the individual who is the subject of the Material. Purchaser agrees not to upload or search the genetic data into any public, private, commercial, or genealogy databases. In the event that Purchaser determines the identity of any individual related to the Material, Purchaser shall not make use of such knowledge, shall safeguard or destroy such information, shall not disclose such information to any other party, and shall notify NIST of such discovery in accordance with the applicable laws and regulations in effect at the time of the discovery.

Use: RM 8048 is provided as frozen stool that should be allowed to thaw at room temperature for no greater than 60 minutes prior to use. After the material is thawed, the entire vial should be used immediately. The contents of the vial should be gently mixed prior to analysis. Precautions should be taken to avoid exposure to strong UV light, direct sunlight and heat.

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Appendix A

Source and Preparation: RM 8048 is created as a pair of distinct human stool samples, corresponding to two dietary donor pools: omnivore and vegetarian. In its final form, the RM 8048 is comprised of homogenized stool from multiple donors resuspended in water to a concentration of 100 mg/mL wet weight. This RM was developed after an appropriate human subject's research determination by NIST.

Omnivore Stool (RM 8048 Part A): The omnivore stool was comprised of five donors for a total of 1,241 g (178 g to 305 g collected per donor). Human fecal material collections were coordinated through BioIVT (Hicksville, NY), under informed consent. Donors were self-reported healthy with no antibiotic use within three months of donation. All donors screened for the following infectious agents via blood draw: hepatitis B/C virus, human immunodeficiency virus (types 1 and 2), West Nile virus, syphilis, and Chagas. All donors were required to complete a food diary corresponding to the week around the donations. Stool donations were collected and stored at –80 ºC and shipped to NIST on dry ice. Samples were combined and cryogenically homogenized, bottled in ~100 g aliquots and stored at –80 ºC. Samples were then shipped on dry ice to BioIVT and stored at –80 ºC. The cryogenically homogenized material was diluted with water to a concentration of 100 mg/mL (cryohomogenized stool/water) and three bacterial strains *Deinococcus radiodurans* (NIST0032), *Brenneria nigrifluens* (NIST0080), and *Deltia acidovorans* (NIST0136) were added to the slurry and homogenized. With constant mixing, a continuous pipettor was used to distribute 1 mL of stool slurry into each sample vial.

Vegetarian Stool (RM 8048 Part B): The vegetarian cohort was comprised of four donors for a total of 1,293 g collected (200 g to 300 g collected per donor). Human fecal material collections were coordinated through BioIVT (Hicksville, NY), under informed consent. Donors were self-reported healthy with no antibiotic use within three months of donation. All donors screened for the following infectious agents via blood draw: hepatitis B/C virus, human immunodeficiency virus (types 1 and 2), West Nile virus, syphilis, and Chagas. All donors were required to complete a food diary corresponding to the week around the donations. Stool donations were collected and stored at –80 ºC and shipped to NIST on dry ice. Samples were combined and cryogenically homogenized, bottled in ~100 g aliquots and stored at –80 ºC. Samples were then shipped on dry ice to BioIVT and stored at –80 ºC. The cryogenically homogenized material was diluted with water to a concentration of 100 mg/mL (cryohomogenized stool/water) and three bacterial strains *Deinococcus radiodurans* (NIST0032), *Brenneria nigrifluens* (NIST0080), and *Deltia acidovorans* (NIST0136) were added to the slurry and homogenized. With constant mixing, a continuous pipettor was used to distribute 1 mL of stool slurry into each sample vial.

Analytical Approach for Metagenomic Identification (NIST): Three replicate vials from each of 10 different boxes were selected for homogeneity and stability testing. For homogeneity testing, one vial from each box was analyzed; for stability, two vials from different boxes were tested at each subsequent time point except for the 12-week time point when vials from six different boxes were tested for the omnivores. For each vial, four replicate DNA extractions were carried out using the Zymo Research Quick-DNA Fecal/Soil Microbe Miniprep Extraction Kit per protocol with the following modification - mechanical disruption was carried out using the Vortex Genie Microtube adapter with the vortex genie set to max rpm for 40 minutes. DNA was eluted and stored at 4 ºC. Following extraction, the V4 region of the16S rRNA genes were amplified by PCR and analyzed by next generation sequencing. Read processing and error correction were carried out using CutAdapt and DADA2 (1.20.0), respectively. Taxonomy was assigned based on the silva database (v138). The non-certified taxa results are comprised of the top 50 sequences identified in the homogeneity analysis.

Analytical Approach for LC-MS/MS Metabolite Identification (NIST): Metabolite identifications were determined by an untargeted liquid chromatography tandem mass spectrometry (LC-MS/MS)-based metabolomics approach. Each phenotypic donor pool (RM 8048 Part A Omnivore, RM 8048 Part B Vegetarian stool) was prepared using a Bligh & Dyer extraction. Ten vials of each stool material were removed from storage at –80 °C and the entire contents were extracted with a 2:2:1.8 solvent system of methanol:chloroform:water. All samples were vortexed for 1 min each, then allowed to sit on ice for 10 min. Samples were centrifuged for phase separation and the polar layer and non-polar layer were each removed and taken to dryness in a vacuum centrifuge, then immediately stored at –80 ºC until analysis. The polar fraction was resuspended in 2 % methanol in water volume fraction prior to LC-MS/MS analysis. The non-polar fraction was resuspended in isopropanol prior to LC-MS/MS analysis. A gradient method with a 0.1 % formic acid in water/0.1 % formic acid in methanol mobile phase and a C18 column was used for polar LC-MS/MS analysis in both positive and negative mode with a data dependent acquisition on two different high resolution MS instruments. For the non-polar fraction, a gradient method with a mobile phase of A: 60:40 acetonitrile:water and B: 90:10 isopropanol:acetonitrile, both with 10 mmol/L ammonium formate and 0.1 % formic acid, and a C30 column were used for non-polar LC-MS/MS analysis in both positive and negative mode using a data dependent acquisition on a high-resolution MS instrument. The resulting tandem MS spectra were searched using HighChem-HighRes, HighChemDP, and NIST spectral library search algorithms with NIST20 and mzVault (version 2019) libraries. Putative metabolite identifications (MSI level 2 [2]) by spectral library matches and scores for each search algorithm, sample preparation, and instrument were filtered (match score ≥65) and combined.

Analytical Approach for NMR Metabolite Identification (NIST Method 1): Metabolite identifications were determined by an untargeted NMR based metabolomics approach. Each phenotypic donor pool (RM 8048 Part A Omnivore, RM 8048 Part B Vegetarian stool) was prepared using a Bligh & Dyer extraction. Ten vials of each stool material were removed from storage at –80 °C and the entire contents were extracted with a 2:2:1.8 solvent system of methanol:chloroform:water. All samples were vortexed for 1 min each then allowed to sit on ice for 10 min. Samples were centrifuged for phase separation and the polar layer and non-polar layer were each removed and taken to dryness in a vacuum centrifuge, then immediately stored at –80 ºC until analysis. The polar fraction was rehydrated in 100 mmol/L sodium phosphate NMR buffer in D_2O containing 1.0 mmol/L sodium 3-Trimethylsilyl 2,2,3,3-d_4 propionate as the chemical shift reference standard. One dimensional ^1H NMR and two dimensional ^1H, ^{13}C-HSQC spectra were collected, and metabolites were assigned based on chemical shift comparisons using reference spectra from the Human Metabolome Database (HMDB), the Biological Magnetic Resonance Bank (BMRB), and the spectral library in Chenomx NMR Analysis software.

Analytical Approach for NMR Metabolite Identification (NIST Method 2): Metabolite identifications were determined by an untargeted NMR-based metabolomics approach. The aqueous portion of 22 vials each phenotypic donor pool (RM 8048 Part A Omnivore, RM 8048 Part B Vegetarian stool) was analyzed after centrifugation for 30 minutes at 14,000 × g at 4 °C, then addition of a 100 mmol/L sodium phosphate buffer, 6.15 mmol/L sodium azide, and sodium 2,2-dimethyl- 2 – silapentane-5-sulfonate-D6 in D_2O. One-dimensional ^1H spectra were collected, and metabolites were assigned based on chemical shift comparisons using reference spectra from the Human Metabolome Database (HMDB), the Biological Magnetic Resonance Bank (BMRB), and the spectral library in Chenomx NMR Analysis software. An additional aqueous portion of a single vial of each phenotypic donor pool (RM 8048 Part A Omnivore, RM 8048 Part B Vegetarian stool) was analyzed after centrifugation for 30 minutes at 14,000 × g at 4 °C, addition of a 100 mmol/L sodium phosphate buffer, and centrifugation for 60 minutes at 10,000 × g at 4 °C with a 3 kDa molecular weight filter. The filtrate was then diluted in D_2O containing 100 mmol/L sodium phosphate NMR buffer containing 0.50 mmol/L sodium 2,2-dimethyl- 2- silapentane-5-sulfonate-D6 (DSS-D6) as the chemical shift reference standard. Two dimensional ^1H, ^{13}C-HSQC spectra were collected, and metabolites were assigned based on chemical shift comparisons using reference spectra from the Human Metabolome Database (HMDB), the Biological Magnetic Resonance Bank (BMRB), and the spectral library in Chenomx NMR Analysis software.

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