

[1]

Supplementary Tables

Supplementary Table 1. Mean concentrations of metabolites (in pmol/mg stool) and mean intra-individual coefficients of variation (CV in %) that were measured in at least one of the tested protocols >LOD.

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
C0	47.62	17.42	17.38	26.19	31.74	12.49	27.22	12.95	39.34	24.41	24.5	23.79	26.23	9.44	42.19	21.46
C7-DC	0.53	35.73	0.23	28.96	0.34	62.53	0.3	34.53	0.41	33.70	0.15	11.02	0.23	43.82	0.38	40.19
C9	0.45	31.00	0.12	5.92	0.14	13.74	0.14	13.27	0.21	19.56	0.09	7.96	0.1	18.62	0.2	17.16
C10	1.39	33.23	0.5	13.49	0.52	19.19	0.51	9.32	0.74	17.71	0.36	12.27	0.4	20.13	0.71	12.07
C12	0.82	24.36	0.34	9.01	0.36	15.06	0.36	10.31	0.45	16.13	0.31	43.42	0.23	18.61	0.46	12.44
C12:1	0.88	27.20	0.41	15.71	0.51	13.57	0.44	10.10	0.65	13.16	0.3	16.58	0.47	14.43	0.64	9.41
C16	0.18	13.74	0.37	28.35	0.38	19.45	0.38	24.30	0.39	6.27	0.41	12.54	0.45	24.57	0.44	26.03
C16:2	0.08	20.27	0.09	18.15	0.12	20.95	0.12	20.44	0.13	10.44	0.12	16.11	0.1	19.49	0.14	16.88
C18	0.09	15.60	0.64	17.50	0.37	15.01	0.55	16.17	0.44	10.24	0.4	12.50	0.59	22.13	0.49	16.22
C18:1	0.1	12.14	0.26	10.12	0.28	21.40	0.31	16.23	0.3	11.67	0.24	15.78	0.3	15.94	0.34	14.45
Trigonelline	3.28	8.34	1.55	28.48	2.29	11.42	2.13	16.83	2.64	17.22	2.05	19.67	1.84	11.01	2.84	15.72
Ala	1041.78	16.11	239.89	34.13	471	25.69	345.11	24.76	509.56	16.17	1625.89	34.07	457	15.60	560.89	30.99
Arg	134.78	20.94	14.6	86.55	56.67	31.35	17.61	53.89	66.57	14.57	365	16.46	137.74	10.77	141.41	41.85
Asn	47.3	30.12	2.94	32.52	7.26	25.57	3.59	34.74	9.57	23.64	108.79	41.74	8.55	10.72	9.06	28.02
Asp	1223.11	15.05	79.14	55.33	652.89	22.67	207.3	39.52	873.44	26.99	881.33	33.66	453.11	18.25	1003.78	28.30
Cys	58.92	14.91	13.32	37.58	37.23	24.24	20.57	27.01	52.1	17.51	31.19	22.37	25.91	15.66	50.78	19.12
Gln	220.78	18.47	28.83	28.46	83.63	16.82	47.99	21.79	83.6	26.24	221.14	35.52	71.76	20.33	97.69	28.08
Glu	5207.11	15.84	507.44	54.52	3912.22	17.69	1946.44	32.95	4124.33	22.24	2814.44	32.34	2561	13.56	5053	25.47
Gly	451.78	15.67	83.11	39.72	247.44	25.40	135.97	30.51	278.89	24.17	479.22	29.07	169.44	14.77	298.11	30.77
His	97.86	15.87	27.47	31.97	52.51	18.94	35.64	20.17	58.39	21.71	66.62	29.79	48.5	11.05	77.08	29.52
Ile	212.56	21.19	39.51	30.94	65.18	36.14	54.48	36.24	67.48	23.80	416.43	34.20	67.29	18.55	75.42	46.28
Leu	366.33	19.45	58.57	38.27	101.6	42.45	82.43	51.18	105.58	30.45	981	41.33	126.9	21.90	118.71	53.44
Lys	1069.89	14.43	169.36	59.03	526	13.62	235.26	44.01	700	16.37	878.11	43.08	400.89	12.24	805.89	15.56

[2]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
Met	197	17.60	33.49	27.18	63.98	19.99	47.97	33.30	61.91	22.99	379.46	32.66	50.92	18.77	64.07	36.43
Phe	187.89	18.01	29.64	31.77	52.23	37.64	42.34	44.79	52.5	26.96	382.56	33.40	55.74	16.41	62.41	49.57
Pro	349	17.17	139	36.46	259.78	20.89	216.94	32.91	247.77	31.72	285.44	25.24	197.72	15.95	312.24	33.25
Ser	298.78	25.40	35.3	30.26	101.03	28.46	57.7	36.39	108.43	27.79	384.56	32.33	64.51	16.08	111.3	39.97
Thr	200.22	14.14	38.76	32.33	87.37	11.31	57.17	21.80	87.17	18.25	265.21	33.83	75.9	13.42	96.93	21.01
Trp	44.2	19.73	9.54	54.06	18.79	29.66	14.17	50.98	15.27	42.54	56.61	28.43	16.65	18.81	20.01	35.86
Tyr	254.11	14.85	68.44	31.70	112.97	29.97	90.49	28.98	113.72	21.68	460.11	31.33	120.81	17.04	142.9	34.00
Val	312.22	15.58	81.7	33.72	133.56	28.13	112.07	29.74	147	22.25	540	33.12	143.11	19.22	160.29	35.22
1-Met-His	3.92	12.65	1.53	32.71	2.77	17.12	2.08	15.69	3.6	20.15	2.35	22.27	2.18	12.34	4.03	20.86
3-Met-His	9.96	10.28	3.62	36.69	7.06	14.47	5.23	19.11	8.92	19.03	6	25.69	6.51	17.01	9.27	19.03
5-AVA	272	18.56	129.98	31.68	232.33	25.75	180.91	19.86	301.22	27.84	208	23.57	251.11	18.69	285.44	25.90
AABA	23.71	11.30	11.29	36.20	19.62	25.91	16.2	24.93	20.22	20.07	25.19	27.55	29.42	21.29	27.06	28.13
Ac-Orn	10.28	15.92	3.26	42.61	5.86	17.33	4.45	26.03	8.01	23.90	5.36	24.55	4.9	11.30	9.23	24.53
ADMA	1.18	8.68	0.48	41.45	0.93	17.81	0.72	22.54	1.15	21.97	0.8	21.66	0.85	14.47	1.27	13.33
alpha-AAA	5.04	10.90	0.88	53.25	3.55	14.30	1.68	36.50	4.88	16.29	3.18	31.55	3	21.38	4.89	19.25
Anserine	3.12	9.69	0.82	41.73	2.12	17.50	1.39	27.98	2.44	23.42	2.18	29.88	2.08	17.52	2.74	26.99
BABA	0.96	14.99	0.61	32.73	0.91	24.37	0.79	25.63	0.99	24.68	0.78	30.69	0.81	14.37	1.16	27.64
Betaine	0	.	1.63	37.17	1.82	22.85	1.16	90.50	0	.	1.35	22.94	2.67	41.64	2.11	23.07
C4-OH-Pro	1.65	11.73	1	11.94	1.33	6.57	1.05	9.70	1.83	15.99	0.93	10.41	0.95	13.18	1.85	7.86
Carnosine	2.97	7.72	1.25	14.22	2.14	11.65	1.42	9.76	2.96	14.16	2.37	19.81	2.25	13.82	3.1	15.68
Cit	503.56	16.71	105.32	29.78	269.78	18.58	164.41	29.51	326.67	19.74	650.56	34.18	164.61	15.44	279.78	25.24
Creatinine	10.66	19.42	14.07	24.70	16.95	35.68	15.79	25.36	20.57	17.30	13.75	20.50	20.63	20.37	18.16	34.51
Cystine	1.27	45.32	0.07	37.85	0.23	37.78	0.09	29.37	0.27	46.97	1.84	50.55	0.27	44.64	0.35	54.93
DOPA	0.66	15.89	0.47	14.58	0.65	11.39	0.56	8.61	0.84	11.32	0.49	13.42	0.4	14.27	0.8	9.31
HArg	0.66	6.36	0.21	27.71	0.46	19.23	0.26	33.42	0.55	22.66	0.52	22.51	0.4	14.81	0.63	19.50
HCys	15.14	8.98	10.82	14.27	12.66	18.81	10.65	13.40	16.53	14.84	16.06	21.17	12.36	19.53	16.38	20.99
Met-SO	10.93	30.81	3.51	33.17	5.94	41.57	4.62	40.99	4.96	28.54	23.32	36.05	11.32	20.70	5.34	53.00
Orn	116.02	13.59	18.96	44.04	42.64	20.03	17.03	49.49	70.34	22.32	50.69	23.40	24.56	12.66	80.04	21.39
PheAlaBetaine	1.02	17.95	0.68	25.96	0.68	21.67	0.76	23.08	0.74	17.83	0.61	24.18	0.59	13.27	0.8	26.41
ProBetaine	8.36	15.65	5.5	18.92	6.92	17.46	6.71	13.64	8.36	16.04	5.63	16.89	5.69	11.70	9.23	12.97

[3]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
Sarcosine	20.55	20.91	9.33	35.33	15.92	20.18	12.76	21.58	21.84	26.69	13.57	13.79	15.68	16.77	21.15	17.68
SDMA	0.71	14.58	0.37	32.18	0.66	26.13	0.49	25.90	0.79	21.26	0.53	20.65	0.66	14.60	0.82	21.97
t4-OH-Pro	25.94	9.59	11.7	25.13	17.91	9.13	13.56	16.77	22.16	21.23	16.3	23.35	15.33	14.42	24.13	14.94
Taurine	41.6	18.44	27.22	29.39	46.49	30.55	39.03	28.81	53.3	22.88	49.45	30.60	52.05	17.66	46.45	36.39
TrpBetaine	0.35	13.82	0.19	20.42	0.23	19.41	0.21	25.37	0.28	21.13	0.25	25.26	0.19	12.84	0.32	29.74
CA	10.32	33.60	15.69	36.54	22.25	55.10	15.67	61.71	21.55	64.14	23.44	47.13	19.47	72.96	18.54	59.91
CDCA	1.24	60.69	12.32	71.26	24.47	90.83	15.72	83.00	11.66	66.55	32.92	93.63	18.37	97.65	11.4	67.64
DCA	21.19	34.20	72.89	32.38	80.49	31.60	73.93	19.85	93.97	19.10	73.54	30.29	76.24	23.17	98.21	31.43
GCA	0.07	57.94	0.32	75.60	0.9	78.49	0.84	68.82	0.8	36.83	0.63	58.79	0.83	46.35	1.58	61.41
GCDCA	0.09	31.33	1.42	84.00	2.8	92.24	1.55	57.03	1.07	33.93	3.51	68.70	3.71	90.30	1.37	35.70
GDCA	0.01	116.77	0.35	70.26	0.65	97.70	0.42	50.00	0.22	50.74	0.93	90.15	0.87	97.32	0.24	37.97
GLCA	0.01	22.12	0.05	26.12	0.05	20.04	0.06	20.19	0.06	17.29	0.06	21.09	0.06	24.47	0.05	20.61
GLCAS	0.01	65.11	0.37	38.34	0.65	54.83	0.82	54.03	0.58	34.84	0.41	35.54	1.46	76.34	0.61	44.35
GUDCA	0.05	72.21	0.03	45.35	0.07	22.92	0.03	65.03	0.06	28.92	0.18	16.37	0.06	48.33	0.06	41.80
TCA	0.21	38.45	1.01	60.47	1.52	84.98	1.73	82.26	1.39	39.33	0.82	86.85	2.35	73.65	1.9	45.47
TCDCa	0.04	28.86	2.73	87.58	4.77	99.18	2.61	69.72	1.56	29.52	1.76	80.22	3.32	83.68	1.93	39.44
TDCA	0.02	19.63	0.46	83.59	1.1	94.00	0.61	81.67	0.26	31.17	0.6	79.70	0.88	89.04	0.29	35.11
TLCA	0.01	59.67	0.13	31.42	0.21	54.73	0.22	54.57	0.17	22.20	0.06	42.78	0.33	39.45	0.16	34.49
TMCA	0.07	32.68	0.06	36.29	0.06	49.56	0.05	41.76	0.08	38.82	0.05	44.25	0.06	49.41	0.08	31.25
beta-Ala	36.71	9.42	13.11	38.04	30.88	18.60	19.4	28.01	32.51	20.68	31.08	30.64	25.21	13.25	37.57	25.75
GABA	22.86	20.37	11.23	37.56	20.44	22.07	15.64	27.65	25.98	25.10	21.04	25.26	22.63	14.79	35.81	46.02
Histamine	5.21	10.30	5.41	13.24	6.19	12.37	5.91	11.32	7.38	9.02	5.31	13.57	5.41	16.08	6.95	12.47
PEA	0.01	21.82	0	106.80	0	.	0	.	0	173.21	0.04	49.63	0.03	72.34	0	.
Putrescine	42.87	17.00	19.56	34.69	27.13	28.64	18.27	46.73	33.46	23.24	23.6	15.29	15.47	18.88	31.27	31.11
Serotonin	0.62	8.21	0.65	20.37	0.78	10.65	0.74	15.20	0.85	16.70	0.59	16.11	0.6	12.18	0.94	16.42
Spermidine	153.33	7.86	37.36	30.92	40.09	19.59	25.76	41.19	45.78	31.49	37.71	25.82	21.48	27.93	40.33	25.28
Spermine	3.49	13.83	1.17	13.75	1.09	11.39	0.95	8.93	1.58	9.39	0.99	11.75	0.67	18.03	1.56	16.19
AconAcid	2.75	11.23	0.23	21.82	0.39	16.86	0.3	16.56	0.44	23.16	0.33	15.36	0.33	14.36	0.48	13.30
DiCA(12:0)	8.43	17.74	2.6	20.14	4.37	12.92	3.64	16.50	4.63	12.22	2.06	11.78	3.4	9.31	5.27	18.36
DiCA(14:0)	0.08	21.98	0.12	26.09	0.12	27.98	0.11	23.84	0.19	17.45	0.13	36.17	0.17	65.74	0.18	12.30

[4]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
OH-GlutAcid	48.71	64.99	0.79	21.83	12.53	32.27	1.98	35.87	4.57	15.89	5.91	57.17	4.54	49.66	4.88	20.74
Suc	1100.67	21.01	94.82	49.03	398.78	41.80	195.21	39.92	602.78	21.89	384.83	30.23	508.89	22.22	601.11	31.91
Cer(d16:1/18:0)	0	.	0.16	121.19	0.02	86.61	0.09	147.06	0.02	173.21	0.16	52.30	0.17	90.74	0.03	173.21
Cer(d16:1/20:0)	0	.	0.08	116.36	0.02	6.32	0.04	91.43	0	.	0.05	116.71	0.06	120.44	0.04	129.99
Cer(d16:1/22:0)	0	.	0.63	43.61	0	.	0.18	123.88	0.12	144.42	0.35	46.95	0.51	40.08	0.1	173.21
Cer(d16:1/23:0)	0	.	0.54	24.74	0	.	0.07	91.84	0.08	131.37	0.33	27.36	0.41	23.81	0.07	88.84
Cer(d16:1/24:0)	0.01	173.21	0.3	31.57	0.01	173.21	0.06	93.74	0.04	173.21	0.13	103.65	0.22	63.64	0.02	173.21
Cer(d18:1/14:0)	0	.	0.26	20.04	0.04	144.34	0.16	93.87	0.09	104.71	0.24	14.01	0.2	100.69	0.09	93.35
Cer(d18:1/16:0)	0.06	89.31	1.81	21.09	0.03	130.34	0.68	32.48	0.56	24.72	1.03	23.22	1.49	37.36	0.6	34.93
Cer(d18:1/18:0(OH))	0	.	0.14	134.42	0	.	0.12	23.39	0.04	173.21	0.15	128.43	0.26	76.62	0.05	173.21
Cer(d18:1/18:0)	0.03	173.21	2.16	28.30	0.01	173.21	0.49	87.78	0.5	73.39	0.79	26.39	1.29	31.89	0.45	67.60
Cer(d18:1/18:1)	0.05	96.81	0.72	20.11	0.08	95.92	0.47	26.54	0.36	21.98	0.58	16.05	0.72	28.20	0.42	24.54
Cer(d18:1/20:0(OH))	0.14	173.21	3.5	91.28	0	.	0.71	173.21	0.66	173.21	2.32	91.27	4.39	73.58	0.66	87.16
Cer(d18:1/20:0)	0.01	173.21	0.24	27.73	0	.	0.06	122.98	0.04	86.82	0.12	19.19	0.19	29.62	0.05	70.97
Cer(d18:1/22:0)	0	.	1.29	25.63	0	.	0.19	106.26	0.2	75.73	0.56	23.00	0.79	31.10	0.1	145.15
Cer(d18:1/23:0)	0	.	1.15	24.78	0	.	0.11	125.06	0.28	25.86	0.47	27.99	0.66	33.25	0.09	145.34
Cer(d18:1/24:0)	0.05	173.21	1.55	16.40	0.02	173.21	0.24	140.04	0.23	89.29	0.61	21.64	0.83	42.64	0.13	99.40
Cer(d18:1/24:1)	0.04	173.21	1.65	24.40	0	.	0.25	86.69	0.33	88.26	0.9	25.56	1.31	34.62	0.14	116.42
Cer(d18:1/25:0)	0.01	173.21	0.71	40.59	0.05	130.68	0.18	105.60	0.26	95.99	0.53	20.55	0.69	32.21	0.09	173.21
Cer(d18:1/26:0)	0.01	173.21	0.08	88.14	0	.	0.05	173.21	0.02	173.21	0.04	94.71	0.09	138.65	0	.
Cer(d18:2/16:0)	0	.	0.18	50.87	0.02	87.12	0.14	104.36	0.15	70.57	0.18	26.14	0.19	20.17	0.13	62.90
Cer(d18:2/18:0)	0	.	0.12	96.16	0.01	93.58	0.08	97.22	0	.	0.1	76.76	0.12	68.60	0.03	173.21
Cer(d18:2/18:1)	0	.	0.03	37.96	0	173.21	0.02	123.30	0.01	173.21	0.03	15.29	0.03	74.32	0.01	129.98
Cer(d18:2/20:0)	0	.	0.01	173.21	0	.	0.01	173.21	0	.	0.02	129.93	0.05	102.30	0	.
Cer(d18:2/22:0)	0	.	0.16	95.31	0	.	0.04	86.80	0.02	173.21	0.06	133.93	0.19	62.49	0	.
Cer(d18:2/23:0)	0	.	0.02	173.21	0	173.21	0	.	0	.	0.05	130.72	0.04	103.26	0	.
Cer(d18:2/24:0)	0	.	0.11	144.35	0	.	0.04	173.21	0	.	0.06	134.85	0.15	92.08	0	.
Cer(d18:2/24:1)	0	.	0.17	15.63	0	.	0.02	173.21	0.02	173.21	0.14	67.97	0.2	28.58	0.01	173.21
CE(14:0)	0.43	145.77	1.34	34.45	0.38	148.60	0.86	66.12	0.4	129.91	0.6	86.89	2.83	110.63	0.33	132.86
CE(15:0)	0.3	130.19	1.21	12.20	0.2	173.21	0.29	130.00	0.61	145.04	0.34	144.53	2.81	93.47	0.35	130.06

[5]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
CE(16:0)	1.89	23.42	7.24	16.90	1.95	25.81	1.79	38.85	2.42	35.38	2.73	28.93	8.46	88.04	2.95	22.41
CE(17:0)	0.54	144.42	0.62	94.66	1.97	98.76	0.84	92.06	0.69	173.21	0.56	108.50	2.34	146.24	1.13	91.44
CE(18:0)	0.46	78.15	2.27	28.05	0.54	42.48	0.55	70.89	0.64	62.54	1.68	56.82	2.19	68.74	0.74	36.07
CE(18:1)	3.42	64.51	14.27	46.86	3.63	45.65	1.58	47.40	1.08	124.44	7.74	32.28	10.54	55.06	3.41	104.63
CE(18:2)	19.17	79.66	10.08	40.16	15.31	62.55	8.86	49.74	7.42	38.42	17.39	55.63	10.66	56.48	20.47	78.91
CE(20:0)	114.61	88.12	1.03	98.99	3.83	144.84	0.76	173.21	4.73	130.39	2.04	115.61	1.9	121.75	26.77	123.08
CE(20:4)	3.2	110.70	1.11	79.45	2.48	62.89	0.98	78.50	1.18	80.52	2.92	55.34	1.23	78.62	2.73	79.71
p-Cresol-SO4	13.52	23.74	4	17.74	4.4	26.11	4.66	29.63	3.96	20.32	4.34	22.38	2.18	17.24	3.71	34.38
DG(14:0_14:0)	0.49	18.31	0.02	128.78	0.04	129.24	0.05	129.03	0.08	23.39	0.03	88.56	0.09	62.24	0.2	98.36
DG(14:1/18:1)	0.11	173.21	0.09	173.21	0	.	0.13	173.21	0.1	173.21	0.6	121.46	0.43	130.40	0.13	173.21
DG(16:0_16:1)	1.53	64.32	1.88	40.56	1.28	45.78	1.66	14.16	1.7	80.34	1.87	51.48	1.63	69.99	1.75	36.06
DG(16:0_18:1)	1.59	72.35	19.62	46.65	1.16	39.82	8.85	70.73	3.87	57.33	14.75	33.92	26.79	40.25	2.96	14.86
DG(16:0_18:2)	1.98	129.56	21.69	33.97	0.51	173.21	9.07	60.23	2.91	92.61	23.34	32.19	24.66	45.44	2.76	43.68
DG(16:1_18:1)	3.41	45.73	4.28	47.51	3.07	61.97	5.96	58.73	6.56	41.36	3.22	22.31	4.12	29.18	3.64	65.86
DG(16:1_18:2)	0	.	1.23	74.85	0.08	173.21	0.6	71.46	0	.	0.81	88.59	1.11	94.52	0.24	87.98
DG(17:0_18:1)	0.25	173.21	1.17	67.29	0.25	173.21	0.5	130.39	0.26	8.39	0.85	95.20	1.37	44.45	0.56	144.43
DG(18:1_18:1)	1.5	33.90	24.06	54.25	0.57	37.73	9.71	66.46	2.25	27.38	23.05	52.76	42.67	72.43	2.55	36.95
DG(18:1_18:2)	6.18	66.92	79.17	48.81	2.21	82.48	26.61	51.26	6.8	44.83	92.59	49.57	78.57	59.03	7.8	45.29
DG(18:1_18:3)	0.74	34.47	7.32	63.15	1.36	50.26	4.64	89.50	1.21	53.50	14.33	72.10	8.1	33.73	1.35	57.22
DG(18:1_20:0)	0.26	173.21	1.51	50.31	0.14	173.21	0.74	93.27	0.47	88.97	1.31	82.24	1.38	41.90	0.23	173.21
DG(18:1_20:4)	0.13	173.21	0.94	107.91	0.06	173.21	0.48	95.39	0.76	131.08	1.02	9.39	1.23	61.50	0.44	144.35
DG(18:1_22:6)	0.73	87.28	1.49	19.77	0.28	104.65	1.1	55.02	1.14	98.07	1.15	71.53	1.59	63.09	0.79	117.21
DG(18:2_18:2)	13.16	120.32	119.43	34.83	3.28	103.06	55.71	38.08	10.47	67.24	154.81	34.65	131.03	38.01	11.1	72.15
DG(18:2_18:3)	0.3	173.21	6.02	63.84	0.63	144.59	4.92	93.55	1.11	118.27	10.77	47.58	4.42	84.24	1.13	111.49
DG(18:2_20:0)	0.05	173.21	0.38	111.92	0.08	130.27	0.22	115.99	0.06	173.21	0.55	65.39	0.48	43.96	0.03	173.21
DG(18:3_18:3)	0.06	97.38	1.88	98.45	0.29	62.11	2.62	135.93	0.43	121.97	6	94.47	2.39	120.11	0.65	130.24
DG(18:3_20:2)	0.53	11.35	0.49	30.00	0.67	12.15	0.72	101.49	0.93	8.85	0.8	27.77	1.01	56.04	0.65	123.14
Cer(d18:0/18:0(OH))	1.12	61.91	2.89	42.50	2.6	35.54	2.24	62.18	3.2	36.38	2.58	20.85	3.03	19.85	2.99	69.74
Cer(d18:0/24:1)	0.16	96.24	0.43	36.80	0.05	173.21	0.24	117.40	0.07	173.21	0.31	34.57	0.34	42.29	0.04	173.21
Arachidonic acid	0.24	25.64	12.88	18.90	15.96	47.37	13.25	14.94	13.75	17.70	19.01	23.06	16.98	32.28	14.47	14.00

[6]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
DHA	0.16	20.80	6.79	21.24	8.93	41.43	7.66	20.04	7.77	28.40	9.37	21.98	9.23	29.06	6.99	21.52
EPA	0.08	33.82	1.42	13.60	2.4	23.07	1.8	16.84	1.8	26.43	2.52	17.57	2.11	26.89	1.92	21.07
FA(12:0)	27.69	14.24	109.58	53.85	64.86	25.01	79.77	26.23	89.26	17.09	116.79	41.01	115.23	39.50	89.42	23.75
FA(14:0)	150	19.64	677.22	42.76	408.67	34.30	488.56	27.35	534.56	18.08	894	50.66	714.11	38.90	479.11	19.13
FA(18:1)	175.11	44.05	2015.22	25.90	1681.56	29.82	1453.56	23.66	1733.89	16.48	5638.67	39.92	5626.33	25.17	1538.67	14.75
FA(18:2)	336.02	39.63	1475.67	21.51	2092.33	29.25	1721.67	23.04	1837.22	10.10	2738.22	35.13	2346.44	25.85	1744.11	21.32
FA(20:1)	4.09	23.33	65.59	35.86	15.72	19.19	27.89	22.66	33.09	20.76	174.41	49.55	166.14	30.04	24.99	26.74
FA(20:2)	2.99	23.68	19.15	24.66	13.57	23.99	15.82	19.11	20.07	10.17	19.32	32.83	21.67	20.51	16.24	23.45
FA(20:3)	1.57	55.15	17.96	38.52	13.84	19.93	17.09	14.26	15.14	29.63	18.82	29.04	19.44	24.46	17.69	24.23
lysoPC a C16:0	0.83	17.12	5.04	26.02	6.6	24.53	5.72	19.07	6.09	24.22	4.84	22.47	8.14	41.55	5.52	26.59
lysoPC a C17:0	0.06	144.75	0.23	21.64	0.21	45.70	0.26	24.26	0.25	64.77	0.18	36.16	0.27	19.65	0.26	38.83
lysoPC a C18:0	0.32	40.98	2.77	18.67	2.14	19.14	2.8	20.85	2.91	23.03	1.87	22.60	3.6	34.72	2.7	23.82
lysoPC a C18:1	0.11	119.76	1.04	48.72	2.31	51.38	1.55	62.64	1.43	31.40	1.01	23.88	9.61	96.31	1.41	43.43
lysoPC a C18:2	0.15	93.66	0.78	66.54	2.66	58.42	1.48	51.29	1.69	56.34	1.08	60.06	1.96	50.42	1.17	40.45
PC aa C24:0	0.07	136.65	0.1	104.48	0.06	63.35	0.04	115.53	0.07	93.16	0.11	101.37	0.04	158.73	0.11	46.37
PC aa C30:0	0.18	13.00	0.67	18.00	0.22	7.30	0.33	8.63	0.39	7.49	0.29	13.18	0.55	24.08	0.42	6.80
PC aa C32:0	0.14	31.09	1.31	25.69	0.14	16.77	0.44	53.95	0.4	32.83	0.44	30.64	1.35	26.11	0.41	52.06
PC aa C32:1	0.04	131.50	0.29	15.75	0.06	144.63	0.24	24.12	0.15	43.65	0.13	45.32	0.51	27.34	0.16	66.22
PC aa C32:2	0.02	173.21	0.11	75.79	0.01	173.21	0.05	144.55	0.05	63.57	0.04	105.98	0.16	29.42	0.1	89.22
PC aa C32:3	0.01	138.12	0.05	94.48	0.01	96.51	0.01	132.57	0.01	89.66	0.01	88.13	0.06	71.74	0.02	144.62
PC aa C34:1	1.43	23.52	3.36	43.67	1.5	34.95	2.1	14.62	1.68	9.38	1.35	42.29	6.91	61.05	2.48	35.01
PC aa C34:2	0.99	82.49	1.83	34.66	0.41	98.45	1.35	37.74	0.76	24.66	0.67	100.35	3.54	43.75	0.59	99.32
PC aa C34:3	0.01	88.86	0.24	39.92	0.06	71.34	0.19	56.71	0.16	110.83	0.14	77.55	0.37	42.86	0.11	26.11
PC aa C34:4	0.01	98.23	0.03	130.95	0.01	136.60	0.02	146.11	0.03	131.10	0.02	116.35	0.05	93.18	0.02	173.21
PC aa C36:1	0.15	47.23	0.76	56.59	0.21	54.44	0.33	24.32	0.19	47.20	0.25	78.42	1.41	39.76	0.23	63.58
PC aa C36:2	2.34	27.08	2.61	54.87	2.24	26.90	1.91	18.27	2.67	16.77	1.95	36.57	19.45	82.77	2.86	19.42
PC aa C36:3	0.08	94.48	1.43	59.36	0.22	82.34	1.05	48.81	0.52	52.68	0.49	106.00	3.13	43.67	0.57	83.67
PC aa C36:4	0.12	108.64	0.91	40.94	0.41	79.19	0.95	27.89	0.49	62.10	0.5	132.89	3.28	56.08	0.24	120.22
PC aa C36:5	0	.	0.24	61.06	0.07	104.95	0.24	80.34	0.24	110.84	0.22	100.83	0.41	45.60	0.04	146.85
PC aa C36:6	0.01	132.08	0.07	112.16	0.05	57.93	0.11	64.93	0.1	157.25	0.07	109.37	0.13	62.60	0.05	71.82

[7]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
PC aa C38:3	0.15	112.48	0.14	53.41	0.05	144.79	0.11	22.88	0.09	74.25	0.23	89.15	0.19	31.32	0.13	99.97
PC aa C38:4	0.28	169.55	0.21	58.60	0.1	124.25	0.12	68.39	0.01	173.21	0.12	99.98	0.38	105.43	0.24	144.91
PC aa C38:5	0.08	173.21	0.12	66.53	0.09	94.13	0.1	41.13	0.1	77.33	0.07	67.42	0.18	47.84	0.17	154.29
PC aa C38:6	0.1	76.37	0.15	24.24	0.1	92.57	0.09	56.95	0.06	63.42	0.1	70.25	0.23	71.96	0.09	106.66
PC aa C42:1	0.02	173.21	0.03	146.19	0.03	124.20	0.02	144.69	0.03	115.75	0.05	64.80	0.04	79.84	0.02	94.20
PC aa C42:2	0.13	23.67	0.14	10.80	0.16	34.18	0.15	18.97	0.2	31.51	0.06	94.80	0.1	43.01	0.17	10.46
PC ae C32:1	0.02	139.60	0.17	24.20	0.01	130.14	0.06	96.31	0.04	130.88	0.08	66.55	0.2	22.53	0.1	80.12
PC ae C32:2	0.11	98.11	0.14	69.62	0.06	86.61	0.12	67.07	0.11	117.28	0.11	68.61	0.16	14.76	0.11	5.70
PC ae C34:0	0.03	116.45	0.23	16.84	0.03	33.97	0.08	61.08	0.08	51.21	0.12	62.56	0.18	28.61	0.09	77.52
PC ae C34:1	0.03	145.08	0.56	18.52	0.08	93.70	0.29	43.68	0.2	22.90	0.25	23.45	0.56	18.03	0.21	96.04
PC ae C34:2	0.03	173.21	0.38	19.53	0.07	48.26	0.22	40.99	0.21	18.70	0.16	42.43	0.51	22.53	0.2	37.56
PC ae C34:3	0.03	127.02	0.16	40.01	0.02	144.46	0.08	78.71	0.07	88.98	0.05	69.64	0.22	33.53	0.07	54.75
PC ae C36:3	0	173.21	0.15	43.56	0.03	124.24	0.11	63.09	0.07	62.85	0.09	102.67	0.18	29.30	0.1	87.73
PC ae C36:4	0.07	101.81	0.17	47.71	0.05	54.20	0.12	26.73	0.05	144.97	0.07	43.59	0.16	47.58	0.11	102.65
PC ae C36:5	0	173.21	0.13	56.90	0.01	130.00	0.07	67.42	0.04	118.62	0.05	102.17	0.12	42.19	0.06	160.46
PC ae C38:3	0.01	173.21	0.09	22.17	0.06	85.76	0.06	93.12	0.04	119.07	0.06	79.32	0.11	53.67	0.09	115.95
PC ae C38:5	0.03	144.62	0.19	24.45	0.11	44.78	0.1	90.25	0.12	13.24	0.08	52.53	0.18	51.83	0.05	145.62
PC ae C38:6	0.02	98.32	0.09	22.10	0.04	71.55	0.08	26.07	0.05	49.77	0.09	36.72	0.1	40.45	0.05	53.90
Hex2Cer(d18:1/16:0)	0.01	173.21	0.84	28.94	0	.	0.25	64.08	0.34	67.72	0.5	17.04	1.19	43.25	0.35	62.93
Hex2Cer(d18:1/18:0)	0.03	87.59	1.19	32.46	0.01	173.21	0.19	129.22	0.28	101.10	0.6	15.44	0.86	29.96	0.31	46.21
Hex2Cer(d18:1/20:0)	0	173.21	0.12	36.29	0	.	0	.	0.02	173.21	0.05	118.08	0.09	71.19	0	.
Hex2Cer(d18:1/22:0)	0.02	173.21	0.52	67.51	0	.	0.04	173.21	0.05	131.36	0.24	42.25	0.44	41.87	0.02	173.21
Hex2Cer(d18:1/24:0)	0	.	0.45	64.24	0.01	173.21	0.03	96.60	0.04	173.21	0.19	73.83	0.37	40.13	0.04	89.40
Hex2Cer(d18:1/24:1)	0	.	0.33	23.46	0	.	0.02	173.21	0.06	173.21	0.16	61.73	0.38	71.47	0.01	173.21
Hex3Cer(d18:1/16:0)	0	.	0.28	89.26	0	.	0	.	0.06	173.21	0.1	131.28	0.24	91.56	0.02	173.21
Hex3Cer(d18:1/24:1)	0.01	.	0.08	173.21	0	.	0	173.21	0.04	.	0.06	173.21	0.16	.	0	173.21
Hex3Cer(d18:1/26:1)	0	173.21	0	134.50	0.02	.	0	.	0	173.21	0.09	89.76	0.02	99.35	0	.
Hex3Cer(d18:1/22:0)	0	.	0.07	.	0	173.21	0.02	.	0	.	0.07	145.54	0	173.21	0.03	.
HexCer(d16:1/22:0)	0	.	0	.	0	.	0.05	140.57	0	.	0.07	139.24	0.03	173.21	0	.
HexCer(d18:1/14:0)	0	.	0.06	144.87	0	.	0.03	173.21	0.09	91.38	0.16	62.80	0.11	96.65	0.05	173.21

[8]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
HexCer(d18:1/16:0)	0	.	1.78	16.48	0.03	173.21	0.6	48.11	1	94.06	1.52	13.93	1.89	30.66	0.78	61.49
HexCer(d18:1/18:0)	0.02	173.21	0.66	51.19	0.01	173.21	0.11	29.93	0.2	130.32	0.41	26.92	0.47	42.69	0.07	131.84
HexCer(d18:1/18:1)	0.02	173.21	0.21	70.81	0.02	173.21	0.12	101.20	0.17	132.09	0.28	49.82	0.36	73.23	0.09	130.91
HexCer(d18:1/20:0)	0.02	173.21	0.38	96.32	0	.	0.04	86.94	0.13	173.21	0.2	116.37	0.3	100.07	0.07	129.94
HexCer(d18:1/22:0)	0.02	173.21	2.11	67.42	0.02	173.21	0.12	173.21	0.15	173.21	1.34	24.07	1.51	39.68	0.14	173.21
HexCer(d18:1/23:0)	0.11	173.21	1.08	66.43	0.04	173.21	0.12	173.21	0.54	136.12	1.03	20.10	0.78	74.01	0.31	149.89
HexCer(d18:1/24:0)	0.01	173.21	0.83	41.33	0.02	173.21	0.03	173.21	0.26	106.03	0.33	92.19	0.48	70.99	0.07	173.21
HexCer(d18:1/24:1)	0.18	129.91	4.88	11.77	0.21	130.28	0.4	94.43	1.32	73.70	2.59	20.57	3.29	33.17	0.86	82.45
HexCer(d18:1/26:0)	0	.	0.18	115.90	0	.	0.03	93.89	0.03	173.21	0.18	43.18	0.24	76.76	0.05	173.21
HexCer(d18:2/16:0)	0	.	0.19	56.08	0.04	94.60	0.07	137.55	0.08	173.21	0.15	116.05	0.27	72.82	0.18	130.26
HexCer(d18:2/18:0)	0.06	91.38	0.04	173.21	0.02	173.21	0	.	0	.	0.04	86.63	0.14	150.27	0	.
HexCer(d18:2/22:0)	0.17	3.84	0.06	173.21	0.06	173.21	0.11	93.74	0.17	102.35	0.16	133.55	0.17	130.47	0.09	173.21
AbsAcid	0.11	27.08	0.16	32.45	0.18	27.66	0.18	12.28	.	29.84	0.12	37.70	0.17	26.15	0.23	28.96
DHEAS	1.89	15.62	3.92	18.26	4.88	22.27	4.52	10.68	.	29.05	4.2	17.99	4.8	42.38	5.05	28.73
3-IAA	67.94	27.82	22.5	26.36	25.63	19.60	26.86	22.70	.	18.64	19.94	20.34	21.04	13.73	31.84	25.86
3-IPA	27.5	19.88	7.94	21.39	9.84	14.28	9.46	15.20	.	15.19	8.33	20.06	9.95	15.42	10.23	16.55
Ind-SO4	0.66	21.85	0.11	43.94	0.34	62.98	0.24	27.68	.	31.59	0.16	36.74	0.29	22.85	0.36	33.50
Indole	1280.44	31.35	575.56	15.84	542.67	19.90	601.67	21.58	.	15.85	367.56	15.90	238.33	10.23	639.11	14.61
Hypoxanthine	243.56	16.11	96.2	23.39	167.8	20.87	129.51	19.47	.	22.00	331.22	23.31	101.73	17.44	142.54	26.64
Xanthine	328.34	27.69	134.56	45.99	253.79	31.33	231.08	48.08	.	23.83	306.68	36.77	166.02	15.96	244.32	38.14
SM (OH) C16:1	0.01	173.21	0.06	107.09	0.02	173.21	0.02	118.77	.	98.96	0.03	97.69	0.06	80.53	0.01	173.21
SM (OH) C22:2	0.04	173.21	0.03	77.51	0.01	173.21	0.01	170.14	.	88.42	0.02	134.85	0.02	69.33	0.06	130.53
SM (OH) C24:1	0.01	173.21	0.05	50.13	0.01	173.21	0.02	131.14	.	92.59	0.03	96.01	0.03	105.18	0.02	144.91
SM C16:0	0.31	158.29	1.9	22.75	0.11	145.66	0.49	48.70	.	29.18	0.9	14.70	1.56	48.66	0.91	38.59
SM C18:0	0.05	134.52	0.49	31.01	0.02	130.06	0.09	68.09	.	102.94	0.19	46.61	0.31	31.09	0.12	54.64
SM C18:1	0.01	94.07	0.02	173.21	0.01	89.03	0.01	88.19	.	173.21	0.03	144.48	0.03	95.14	0	173.21
SM C22:3	0.02	173.21	0.02	94.96	0.06	149.34	0.13	81.82	.	159.14	0.04	138.93	0.07	107.55	0.14	104.44
SM C24:1	0.07	131.48	0.2	54.32	0.06	119.05	0.06	105.02	.	50.53	0.11	84.67	0.18	58.98	0.14	72.13
H1	3171.89	17.04	881.56	14.95	1369.56	19.35	1023.56	13.27	.	20.63	2703.89	18.77	666.44	15.54	1248.78	11.50

[9]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
TG(14:0_34:1)	0.05	173.21	2.29	105.32	0.03	173.21	0.16	173.21	0.11	86.62	1.21	98.09	5.45	62.49	0.4	148.55
TG(14:0_34:2)	0.12	86.92	0.88	92.70	0.03	173.21	0	.	0	.	0.58	71.79	1.91	50.73	0.18	173.21
TG(14:0_36:1)	0	.	0.34	155.63	0.04	173.21	0	.	0	.	0.04	173.21	1.06	85.38	0.05	173.21
TG(14:0_36:2)	0.15	132.89	1.64	84.52	0.05	99.76	0.04	173.21	0	.	0.98	43.27	4.09	89.61	0	.
TG(14:0_36:3)	0.23	146.76	0.61	89.77	0.04	173.21	0.05	173.21	0.03	173.21	0.75	64.84	2.06	81.90	0	.
TG(14:0_36:4)	0.17	173.21	0.41	97.57	0.02	173.21	0	.	0	.	0.52	146.79	1.06	94.72	0.02	173.21
TG(16:0_28:1)	0	.	1.39	115.82	0.04	173.21	0.19	173.21	0.05	173.21	0.93	71.87	2.79	79.74	0.11	173.21
TG(16:0_28:2)	0	.	0.46	140.08	0	.	0.2	173.21	0.17	173.21	0.26	130.08	0.7	134.53	0.14	173.21
TG(16:0_30:2)	0	.	1.52	109.67	0	.	0.27	95.44	0.24	173.21	0.89	129.86	3.48	97.26	0.1	173.21
TG(16:0_32:0)	4.35	13.61	3.87	13.22	3.89	14.86	4.09	22.04	5.37	18.33	7.08	25.72	12.58	47.62	5.35	12.33
TG(16:0_32:1)	0.49	107.91	3.37	60.08	0.31	105.21	0.52	96.35	0.43	145.32	1.73	27.36	5.96	99.27	1.01	112.66
TG(16:0_32:2)	0.23	117.44	2.1	59.14	0.21	89.78	0.21	126.68	0.03	173.21	0.9	51.57	2.63	73.28	0.32	140.80
TG(16:0_33:1)	0.14	173.21	0.7	90.20	0.17	173.21	0.53	105.32	0.61	94.86	0.38	101.65	1.05	52.61	0.91	52.09
TG(16:0_33:2)	0.08	89.41	0.41	95.45	0	.	0.15	173.21	0	.	0.24	104.77	0.89	57.65	0.13	173.21
TG(16:0_34:0)	2.9	16.54	3.1	34.30	2.69	22.03	2.95	10.49	3.93	13.57	2.62	22.25	8.3	99.77	3.54	16.09
TG(16:0_34:1)	2.16	59.06	28.75	73.97	1.24	35.57	1.75	50.91	1.94	119.96	16.26	28.63	59.71	83.12	2.69	52.26
TG(16:0_34:2)	2.49	96.46	24.73	72.13	0.73	104.92	0.74	91.71	0.98	60.29	17.87	32.30	41.75	86.11	1.83	75.96
TG(16:0_34:3)	0	.	2.64	67.94	0.04	173.21	0.06	173.21	0.1	173.21	4.02	99.74	3.4	81.82	0.18	173.21
TG(16:0_35:1)	0.07	173.21	0.61	39.09	0.08	173.21	0.11	173.21	0.04	173.21	0.39	106.75	0.88	104.14	0.3	102.52
TG(16:0_35:2)	0.02	173.21	0.46	72.37	0	.	0.06	173.21	0.06	173.21	0.24	133.28	0.89	115.96	0.09	173.21
TG(16:0_35:3)	0	.	0.18	133.26	0	.	0.02	173.21	0	.	0.36	54.21	0.28	120.13	0	.
TG(16:0_36:2)	4.61	57.36	63.53	86.64	1.7	33.63	1.76	53.93	2.38	50.76	43.77	35.64	192.43	107.23	4.71	76.86
TG(16:0_36:3)	7.96	81.66	63.27	67.62	1.54	66.59	1.42	34.93	2.21	95.31	61.46	24.19	118.09	110.27	5.52	71.43
TG(16:0_36:4)	8.36	64.98	46.7	49.27	0.67	94.64	0.89	71.92	1.32	143.72	60.3	35.50	85.73	68.60	3.74	61.51
TG(16:0_36:5)	0	.	5.65	85.88	0	.	0.04	173.21	0.38	86.66	13.43	77.35	6.21	50.18	0.4	147.69
TG(16:0_36:6)	0.14	173.21	5.57	122.43	0.13	173.21	0.48	102.57	0.81	72.46	21.94	55.08	10.46	44.74	0.76	121.15
TG(16:0_37:3)	0	.	0.5	134.16	0	.	0	.	0	.	0.66	44.93	1.03	72.35	0	.
TG(16:0_38:1)	0	.	0.48	73.70	0	.	0	.	0.03	173.21	0.34	105.12	0.94	114.69	0.03	173.21
TG(16:0_38:2)	0	.	0.88	115.50	0	.	0.02	173.21	0	.	0.68	96.33	1.55	115.09	0.05	173.21
TG(16:0_38:3)	0.08	173.21	0.6	91.36	0.14	103.04	0.13	173.21	0.13	144.41	0.53	79.70	1.01	77.87	0.09	173.21

[10]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
TG(16:1_32:1)	0.16	173.21	2.27	33.22	0.3	86.63	0.19	129.96	0.19	173.21	0.88	117.98	1.77	74.36	1.37	132.28
TG(16:1_32:2)	0.12	87.43	4.15	74.88	0.04	173.21	0.4	122.30	0.09	173.21	1.62	75.30	2.7	97.09	0.49	173.21
TG(16:1_34:1)	0.31	173.21	2.86	73.87	0.45	94.38	0.38	118.61	0.09	173.21	1.34	47.82	3.9	81.72	0.8	119.52
TG(16:1_34:2)	0.21	173.21	5.47	66.37	0	.	0.12	116.54	0.07	173.21	2.28	47.15	4.09	76.15	0.45	147.11
TG(16:1_34:3)	0.03	173.21	0.63	23.42	0	.	0.03	173.21	0	.	0.26	130.61	0.56	61.34	0.16	123.20
TG(16:1_36:1)	0	.	1.46	78.98	0	.	0.06	173.21	0.08	173.21	0.55	74.69	2.33	78.23	0.16	173.21
TG(16:1_36:2)	0.2	173.21	3.56	83.85	0.09	173.21	0.09	173.21	0.16	173.21	1.95	45.08	11.16	112.81	0.35	173.21
TG(16:1_36:3)	0.44	138.54	2.13	69.36	0.1	173.21	0.05	99.27	0.06	90.47	1.95	28.03	3.94	93.94	0.26	134.63
TG(16:1_36:4)	0.26	131.72	1.41	78.25	0	.	0	.	0.02	173.21	1.59	67.56	2.18	100.60	0.07	173.21
TG(16:1_38:3)	0	.	0.29	62.06	0	.	0	.	0	.	0.23	129.97	0.6	131.83	0.03	173.21
TG(16:1_38:4)	0.04	173.21	0.38	87.00	0	.	0	.	0	.	0.55	15.70	0.7	107.44	0.05	173.21
TG(16:1_38:5)	0	.	0.22	57.93	0	.	0	.	0	.	0.35	11.96	0.43	110.67	0	.
TG(17:0_36:3)	0.02	173.21	0.43	115.64	0	.	0	.	0	.	0.45	118.56	0.94	128.08	0.11	173.21
TG(17:0_36:4)	0.08	130.21	0.28	130.31	0	.	0.02	173.21	0	.	0.47	99.81	0.66	132.53	0	.
TG(17:1_34:2)	0.03	173.21	0.27	91.50	0.06	173.21	0	.	0.08	173.21	0	.	0.4	114.53	0.09	173.21
TG(17:1_36:3)	0.02	173.21	0.27	86.93	0	.	0	.	0	.	0.12	173.21	0.7	132.09	0	.
TG(17:1_36:4)	0.07	173.21	0.25	130.67	0	.	0	.	0	.	0.31	13.41	0.45	122.97	0	.
TG(17:2_36:2)	0	.	0.11	93.54	0	.	0	.	0	.	0.21	24.33	0.63	109.11	0	.
TG(17:1_36:3)	0.02	173.21	0.2	88.70	0	.	0.02	173.21	0	.	0.33	106.35	0.52	84.20	0	.
TG(17:2_36:4)	0	.	0.4	108.12	0.03	173.21	0.1	133.11	0	.	0.43	117.57	0.57	117.17	0	.
TG(18:0_30:1)	0	.	0.81	138.72	0	.	0	.	0.04	173.21	0.48	65.48	1.99	133.76	0.05	173.21
TG(18:0_32:1)	0	.	1.08	118.12	0	.	0	.	0.09	173.21	0.52	95.36	1.35	75.53	0.14	173.21
TG(18:0_32:2)	1.39	123.46	1.82	37.91	1.14	93.26	1.37	99.04	1.58	126.20	1.33	67.16	2.36	39.14	1.71	103.34
TG(18:0_34:2)	1.04	121.38	9.73	68.15	0.04	173.21	0.13	138.19	0.29	96.14	8.4	59.52	15.73	76.88	0.44	146.33
TG(18:0_34:3)	0.04	173.21	0.8	118.43	0	.	0.06	173.21	0.04	173.21	1.47	132.51	1.08	91.47	0	.
TG(18:0_36:1)	0.22	130.51	6.01	80.69	0.05	173.21	0.03	173.21	0.2	145.03	4.2	30.17	13.42	93.72	0.12	173.21
TG(18:0_36:2)	1.76	85.98	24.72	83.52	0.36	49.84	0.39	123.69	0.65	123.98	20.12	37.64	68.2	105.62	1.65	96.14
TG(18:0_36:3)	3.02	112.80	28.9	64.40	0.36	94.92	0.3	137.24	1.07	99.30	33.69	34.48	47.6	105.42	2.21	120.71
TG(18:0_36:4)	3.55	70.76	21.42	47.65	0.16	133.30	0.49	139.56	1.05	116.74	33.58	63.22	38.43	64.93	1.84	81.26
TG(18:0_36:5)	0	.	1.89	110.43	0	.	0	.	0.16	120.49	4.81	141.73	1.97	115.99	0.26	129.08

[11]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
TG(18:1_26:0)	0.12	173.21	13	63.89	0.32	130.02	2.46	92.14	1.82	42.75	7.77	29.66	26.16	56.17	0.98	99.11
TG(18:1_28:1)	0.04	173.21	1.71	90.42	0.12	131.34	0.33	123.76	0.27	148.30	1.13	67.36	3.18	93.24	0.09	173.21
TG(18:1_30:0)	0.19	130.72	3.73	71.82	0.14	95.13	0.37	124.24	0.54	91.46	1.89	74.09	7.36	90.97	0.62	121.23
TG(18:1_30:1)	0.17	173.21	5.97	74.16	0.04	173.21	0.72	115.15	0.18	173.21	3.3	50.46	14.72	63.37	0.38	153.01
TG(18:1_30:2)	0.03	173.21	1.26	100.79	0	.	0.22	173.21	0.11	87.85	0.79	99.38	3.34	85.54	0	.
TG(18:1_32:0)	1.57	27.21	11.33	74.84	1.24	42.57	1.21	17.45	2	23.45	7.17	19.01	23.15	87.31	2.24	29.81
TG(18:1_32:1)	0.5	160.93	4.82	72.18	0.34	117.50	0.38	125.39	0.33	144.81	2.03	66.04	10.86	84.98	0.85	122.85
TG(18:1_32:2)	0.34	98.17	2.91	71.10	0.04	173.21	0.09	173.21	0.05	173.21	1.58	43.54	3.43	63.73	0.3	136.09
TG(18:1_32:3)	0	.	0.1	173.21	0.03	173.21	0	.	0.03	173.21	0.41	61.32	0.17	173.21	0	.
TG(18:1_33:0)	0.05	173.21	0.38	66.66	0.02	173.21	0.02	173.21	0	.	0.17	91.74	0.84	69.53	0.18	137.84
TG(18:1_33:1)	0	.	0.81	115.63	0.03	173.21	0.04	173.21	0.24	145.54	0.19	144.83	1.55	65.70	0.31	173.21
TG(18:1_33:2)	0	.	0.42	87.23	0	.	0.03	173.21	0	.	0.43	94.50	0.78	76.00	0.14	173.21
TG(18:1_34:1)	6.29	73.76	98.63	76.72	2.39	42.13	2.95	63.25	4.37	58.26	60.99	34.52	319.18	109.51	7.65	83.15
TG(18:1_34:2)	7.48	77.01	61.19	75.97	1.33	72.03	1.41	63.32	1.76	61.52	53.94	27.52	122.16	107.74	5.03	72.25
TG(18:1_34:3)	0.85	92.60	6.13	49.62	0.11	173.21	0.39	118.52	0.47	134.88	12.2	62.11	10.92	84.36	0.84	54.23
TG(18:1_34:4)	0.08	87.93	0.35	117.67	0.04	173.21	0.03	173.21	0.12	86.62	0.71	66.96	0.76	79.94	0.03	173.21
TG(18:1_35:2)	0	.	1.5	83.54	0	.	0	.	0	.	0.87	56.59	3.97	108.72	0.11	173.21
TG(18:1_35:3)	0	.	0.44	116.99	0	.	0	.	0.01	173.21	0.37	121.75	0.8	115.22	0.07	173.21
TG(18:1_36:0)	0.4	62.81	5.91	79.15	0.45	45.75	0.29	50.79	0.56	90.44	4.17	36.07	16.32	103.86	0.74	57.60
TG(18:1_36:1)	3.6	55.80	64.64	77.35	0.82	68.72	1.32	45.65	3.03	72.96	43.71	41.77	252.6	120.27	4.54	63.76
TG(18:1_36:2)	16.04	68.16	304.54	75.19	3.36	29.53	8.2	88.58	14.26	85.31	203.51	50.99	1408.61	122.84	19.72	80.92
TG(18:1_36:3)	21.05	49.38	218.5	76.43	1.94	34.51	2.84	57.13	6.99	84.72	224.62	50.95	454.12	119.58	14.08	95.22
TG(18:1_36:4)	22.9	69.24	125.47	47.41	1.03	66.97	2.52	51.40	5.27	73.32	177.95	40.39	236.54	98.83	9.1	65.28
TG(18:1_36:5)	1.15	127.28	10.05	52.70	0.19	130.25	0.32	119.58	1.04	133.70	23.26	50.43	16.84	48.73	1.22	123.83
TG(18:1_36:6)	0.19	173.21	5.28	138.94	0.09	173.21	0.22	173.21	1.56	130.91	25.91	73.24	11.31	67.00	1.06	154.08
TG(18:1_38:7)	0	.	0.18	173.21	0	.	0	.	0	.	0.18	109.37	0.43	144.47	0	.
TG(18:2_28:0)	0	.	2.22	112.65	0.05	91.96	0.21	173.21	0	.	1.06	105.69	4.28	112.16	0.12	173.21
TG(18:2_30:0)	0.04	173.21	0.91	116.88	0.14	129.92	0.1	173.21	0.11	173.21	0.57	100.21	2.06	94.12	0.14	97.45
TG(18:2_30:1)	0.03	173.21	1.25	116.45	0.11	173.21	0.31	150.92	0	.	0.82	101.64	3.37	99.20	0.17	173.21
TG(18:2_32:0)	1.98	67.19	9.76	65.55	1.25	73.08	1.17	52.61	1.05	74.31	7.33	17.53	16.32	77.15	1.7	48.14

[12]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
TG(18:2_32:1)	0.08	173.21	1.47	60.10	0.03	173.21	0.08	173.21	0.14	173.21	1.14	33.04	3.06	91.06	0.45	154.76
TG(18:2_32:2)	0.3	173.21	1.26	86.14	0	.	0.07	173.21	0	.	1.11	99.75	2.28	63.30	0.09	173.21
TG(18:2_33:1)	0	.	0.2	97.56	0.03	173.21	0	.	0.03	173.21	0.27	106.04	0.73	100.27	0.16	131.28
TG(18:2_33:2)	0	.	0.5	108.80	0	.	0	.	0.03	173.21	0.55	120.40	0.68	98.83	0.02	173.21
TG(18:2_34:0)	1.43	112.89	11.03	65.69	0.15	173.21	0.19	96.59	0.36	116.42	10.21	29.27	18.51	92.37	0.77	84.60
TG(18:2_34:1)	8.06	103.50	61	68.45	1.38	80.84	1.1	69.09	1.76	101.72	58.47	29.89	108.04	108.04	4.95	69.34
TG(18:2_34:2)	13.39	60.45	71.79	46.06	1.4	60.98	1.66	79.63	2.42	75.70	80.96	33.66	127.17	74.22	5.52	72.61
TG(18:2_34:3)	0.48	154.41	5.84	79.48	0.11	130.89	0.19	144.38	0.4	120.49	10.82	60.38	7.25	57.91	0.24	173.21
TG(18:2_34:4)	0	.	0.63	114.92	0.03	173.21	0	.	0.07	173.21	1.58	77.43	1.02	108.92	0.04	173.21
TG(18:2_35:1)	0.07	88.15	1.01	85.67	0	.	0	.	0	.	0.94	58.33	1.6	96.67	0.04	173.21
TG(18:2_35:2)	0	.	0.98	109.95	0.03	173.21	0	.	0	.	0.83	89.81	1.57	93.28	0.04	173.21
TG(18:2_35:3)	0	.	0.42	135.07	0	.	0	.	0	.	0.42	123.77	0.64	125.91	0.03	173.21
TG(18:2_36:0)	0.55	145.19	4.69	92.37	0.06	86.69	0	.	0.1	173.21	4.62	65.58	7.5	94.43	0.32	149.23
TG(18:2_36:1)	4.2	69.58	38.81	75.47	0.36	118.61	0.38	122.34	1.29	97.90	42.09	43.23	67.91	111.59	2.34	139.44
TG(18:2_36:2)	19.32	56.86	152.22	70.54	1.3	56.16	2.42	55.55	4.25	103.35	172.22	44.34	299.73	114.24	10.23	75.51
TG(18:2_36:3)	42.43	68.17	235.73	51.64	1.44	143.32	4.3	74.33	6.87	76.78	297.56	45.31	418.71	100.05	15.13	79.33
TG(18:2_36:4)	41.24	57.49	176.25	41.99	1.33	73.98	5.41	69.46	5.49	91.25	252.95	45.73	337.38	56.14	10.43	81.06
TG(18:2_36:5)	0.11	173.21	11.82	82.26	0.1	173.21	0.75	85.96	1.31	126.80	26.87	54.98	13.58	43.29	1.3	128.53
TG(18:2_38:4)	0	.	0.32	110.00	0	.	0	.	0	.	0.5	66.68	0.33	135.04	0	.
TG(18:3_32:0)	0.11	131.61	0.87	102.72	0.03	173.21	0.04	173.21	0	.	1.39	91.41	0.8	122.53	0.19	138.77
TG(18:3_34:0)	0.16	45.59	0.65	97.10	0	.	0	.	0	.	2.27	129.71	1.2	113.31	0.05	173.21
TG(18:3_34:1)	0.36	112.16	5.22	63.11	0.05	173.21	0	.	0.47	144.69	13.22	72.74	8.85	58.48	0.54	108.93
TG(18:3_34:2)	0	.	6.02	82.31	0.09	90.08	0.11	173.21	0.38	87.49	13.94	75.73	6.38	50.20	0.41	92.88
TG(18:3_34:3)	0.04	173.21	7.73	124.19	0	.	0.25	173.21	0.98	86.91	31.13	123.08	13.75	80.95	0.79	106.08
TG(18:3_35:2)	0.02	173.21	0.14	138.55	0	.	0	.	0	.	0.31	96.39	0.21	145.62	0	.
TG(18:3_36:1)	0.33	86.67	3.06	103.96	0	.	0	.	0.63	133.50	7.79	120.27	4.68	110.08	0.53	147.68
TG(18:3_36:2)	1.14	121.70	10.52	43.80	0.07	92.00	0.32	117.27	1.38	136.96	25	41.78	16.9	81.72	1.21	146.26
TG(18:3_36:3)	1.15	128.45	12.63	66.09	0.28	150.26	0.68	97.04	1.81	88.23	34.48	68.42	20.22	47.97	1.7	68.45
TG(18:3_36:4)	0.31	144.38	15.89	85.39	0.24	173.21	0.86	122.79	3.33	130.54	62.32	56.16	26.68	47.12	2.67	132.21
TG(20:0_32:4)	0	.	0.3	130.12	0	.	0	.	0	.		95.50	0.62	136.34	0	.

[13]

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV -3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
TG(20:0_34:1)	0.25	86.67	0.84	58.85	0.1	96.33	0.12	86.85	0.45	127.62	0.58	91.84	1.56	80.40	0.12	173.21
TG(20:1_34:1)	0.11	173.21	0.57	117.03	0.03	173.21	0	.	0.04	173.21	0.39	56.80	0.93	103.76	0.03	173.21
TG(20:1_34:2)	0.15	173.21	0.33	87.30	0	.	0	.	0	.	0.46	59.95	0.94	97.39	0.07	87.78
TG(20:2_34:2)	0	.	0.25	86.92	0	.	0	.	0	.	0.38	15.36	0.64	108.79	0	.
TG(20:2_34:3)	0	.	0.38	57.32	0	.	0	.	0	.	0.3	90.62	0.54	111.30	0	.
TG(20:2_34:4)	0	.	0.37	26.77	0	.	0	.	0	.	0.44	9.39	0.55	47.05	0	.
TG(20:3_32:2)	1.03	54.40	0.6	16.28	0.88	104.50	0.89	92.84	0.75	130.18	0.75	99.41	0.93	21.47	0.71	16.67
TG(20:3_34:2)	0	.	0.26	89.62	0	.	0	.	0	.	0.31	95.78	0.44	53.66	0	.
TG(20:3_34:3)	0	.	0.24	87.00	0	.	0	.	0	.	0.41	88.32	0.4	99.18	0	.
TG(20:5_36:3)	0	.	0.08	173.21	0.02	173.21	0	.	0	.	0.31	106.05	0.4	115.73	0.04	173.21
TG(22:2_32:4)	0.16	154.06	0.48	127.85	0.04	173.21	0.2	129.94	0.38	94.64	0.67	101.53	0.92	81.64	0.13	92.59
Choline	22.1	12.44	8.82	22.38	14.9	19.62	12.94	11.30	15.2	19.15	20.32	23.97	13.08	12.33	17.57	32.29

Concentrations below the LOD are marked in grey.

Abbreviations: 3-IAA, 3-Indoleacetic acid; 3-IPA, 3-Indolepropionic acid; 5-AVA, 5-Aminovaleric acid; AABA, alpha-Aminobutyric acid; Abs Acid, Abscisic acid; AconAcid, Aconitic acid; Ac-Orn, Acetylmethionine; ADMA, Asymmetric dimethylarginine; Ala, Alanine; alpha-AAA, alpha Amino adipic acid; Arg, Arginine; Asn, asparagine; Asp, aspartate; BABA, beta-Aminobutyric acid; betaAla, beta-Alanine; C0, Carnitine; C7-DC, Pimeloylcarnitine; C8, Octanoylcarnitine; C9, Nonanoylcarnitine; C10, Decanoylcarnitine; C10:1, Decenoylcarnitine; C10:2, Decadienoylcarnitine; C12, Dodecanoylcarnitine; C16, Hexadecanoylcarnitine; C16-1OH, Hydroxyhexadecanoylcarnitine; C16:2, Hexadecadienoylcarnitine; C18, Octadecanoylcarnitine; CA, Cholic acid; CDCA, Chenodeoxycholic acid; CE, Cholesteryl ester; Cer, Ceramide; Cit, Citrulline; Cys, Cysteine; DCA, Deoxycholic acid; DG, Diglycerides; DHA, Docosahexaenoic acid; DHEAS, Dehydroepiandrosteron sulfate; DiCA(12:0), Dodecanedioic acid; DOPA, Dihydroxyphenylalanine; EPA, Eicosapentaenoic acid; FA, Fatty acid; Fa(12:0), Lauric acid; FA(14:0), Myristic acid; FA(18:1), Octadecenoic acid; FA(18:2), Octadecadienoic acid; FA(20:1), Eicosenoic acid; FA(20:2), Eicosadienoic acid; FA(20:3), Eicosatrienoic acid; H1, Hexoses (including glucose); GABA, gamma-Aminobutyric acid; GCA, Glycocholic acid; GDCA, Glycodeoxycholic acid; GLCA, Glycolithocholic acid; GLCAS, Glycolithocholic acid sulfate; Gln, Glutamine; Glu, Glutamate; Gly, Glycine; GUDCAS, Glycoursodeoxycholic acid; HArg, Homoarginine; HCys, Homocysteine; HexCer, Hexosylceramide; Hex2Cer, Dihexosylceramide; Hex3Cer, Trihexosylceramide; His, Histidine; Ile, Isoleucine; Leu, Leucine; lysoPC, Lysophosphatidylcholine; Met, Methionine; Met-So, Methionine sulfoxide; OH-GlutAcid, 3-Hydroxyglutaric acid; Orn, Ornithine; PC, Phosphatidylcholine; p-cresol SO4, p-Cresol sulfate; PEA, Phenylethylamine; Phe, Phenylalanine; Pro, Proline; SDMA, Symmetric dimethylarginine; Ser, Serine; SM, Sphingomyelin; Suc, Succinic acid; t4-OH-Pro, trans-4-Hydroxyproline; TCA, Taurocholic acid; TCDCA, Taurochenodeoxycholic acid; TDCA, Taurodeoxycholic acid; TG, Triglyceride; Thr, Threonine; TLCA, Tauroolithocholic acid; TMAO, Trimethylamine N-oxide; TMCA, Taumurocholic acid; Trp, Tryptophan; Tyr, Tyrosine; Val, Valine.

[14]

Supplementary Table 2. Mean concentrations of metabolite sums and ratios (metabolism indicators; in pmol/mg stool) and mean coefficients of intra-individual variation (CVs in %) for metabolite sums and ratios that were measured in at least one of the tested protocols >LOD.

Protocol Metabolite	1		2		3		4		5		6		7		8	
	mean	CV -1	mean	CV -2	mean	CV-3	mean	CV -4	mean	CV -5	mean	CV -6	mean	CV -7	mean	CV -8
CACT Deficiency (NBS)	183.51	14.54	28.92	11.67	59.53	15.70	56.98	12.38	63.32	21.71	45.09	23.69	47.48	17.23	59.24	17.16
CPT-1 Deficiency (NBS)	0.01	10.74	0.09	12.16	0.04	16.38	0.06	11.87	0.04	21.60	0.06	25.64	0.09	18.00	0.04	20.34
Asn Synthesis	0.04	28.87	0.06	58.47	0.01	30.41	0.03	29.53	0.01	17.59	0.11	17.95	0.02	11.99	0.01	20.01
Cys Synthesis	0.14	30.83	0.2	32.19	0.27	37.00	0.24	32.71	0.32	16.05	0.06	13.43	0.25	10.23	0.34	38.00
DLD (NBS)	1.88	11.89	5.14	30.63	5.08	29.74	5.39	33.61	5.04	24.91	0.92	19.33	3.84	7.65	5.37	32.00
Fischer Ratio	1.83	7.24	1.68	15.06	1.68	10.10	1.74	11.11	1.77	9.26	2.07	7.24	1.78	5.39	1.58	13.03
Glutaminase Activity	23.49	16.29	18.82	34.67	40.17	11.07	32.33	23.94	50.09	14.74	13.19	18.56	33.31	18.30	49.66	14.61
Gly Synthesis	1.6	12.64	2.46	30.91	2.56	21.56	2.47	11.86	2.66	14.46	1.34	6.69	2.89	9.71	2.79	24.81
GSH Constituents	5717.89	15.40	604	51.53	4196.78	18.13	2102.78	31.59	4455.22	22.29	3324.89	31.78	2756.44	13.57	5401.89	25.52
MTHFR Deficiency (NBS)	1.04	6.41	1.21	8.72	1.24	18.58	1.18	15.04	1.23	10.01	0.96	6.65	0.9	9.55	1.09	16.76
PKU (NBS)	1.36	6.39	2.44	17.25	2.23	17.49	2.26	20.56	2.25	11.53	1.21	8.68	2.22	2.85	2.45	21.27
Ratio of Non-Essential to Essential AAs	3.5	6.50	2.61	12.85	5.26	8.90	4.66	11.85	5.32	9.80	2.01	10.47	4.8	5.25	5.37	12.95
Sum of AAs	11975.44	14.81	1699.78	40.95	7043	19.83	3771.22	28.50	7763.33	20.98	10584.13	17.17	5253.33	13.45	9262.33	25.21
Sum of Aromatic AAs	486.22	16.10	107.63	32.23	183.96	31.62	147	32.41	181.56	23.04	899.22	31.66	193.11	16.72	225.33	36.76
Sum of Branched-Chain AAs	891.44	17.57	179.81	33.81	300.22	33.60	249	37.76	320.22	25.31	1937.44	37.60	337	20.02	354.44	43.96
Sum of Essential AAs	2688.44	15.62	488	37.82	1101.11	18.86	681.56	32.02	1295.22	18.83	3538.63	17.41	985.89	14.77	1480.89	24.43
Sum of Non-Essential AAs	9287	14.82	1211.67	43.10	5941.89	19.35	3089.89	28.97	6468	22.09	7657.22	31.75	4267.33	13.64	7781.56	26.07
Sum of Solely Glucogenic AAs	9840.44	14.63	1324.67	41.96	6166.11	19.40	3252.22	28.02	6709	21.78	8448.78	31.97	4465.22	13.61	8037.22	25.87
Sum of Solely Ketogenic AAs	1436.33	15.70	227.98	48.32	627.56	15.75	317.33	39.01	805.56	17.75	1761.13	17.14	527.78	13.78	924.44	19.64
Sum of Sulfur-Containing AAs	255.78	13.02	46.82	27.12	101.16	17.99	68.6	26.21	113.97	19.38	410.78	32.08	76.78	16.16	115.07	22.91
Valinemia (NBS)	1.69	10.48	2.76	12.65	2.73	15.87	2.9	15.96	2.8	8.20	1.5	2.63	2.69	3.36	2.71	17.65
Cit Synthesis	6.8	11.48	9.83	15.93	9.81	17.91	17.29	23.57	7.97	14.88	17.76	16.49	12.42	13.76	5.94	11.57
OTC Deficiency (NBS)	0.26	10.72	0.2	16.27	0.25	17.86	0.16	25.92	0.27	14.22	0.16	15.43	0.21	13.47	0.32	10.99
Ratio of HArg to ADMA	0.63	6.76	0.48	24.01	0.48	10.05	0.34	15.85	0.48	7.76	0.66	13.21	0.44	7.00	0.51	10.09
Ratio of HArg to SDMA	0.98	13.88	0.56	20.46	0.68	11.81	0.5	21.97	0.68	9.87	0.95	14.38	0.58	4.26	0.76	18.95

Protocol Metabolite	[15]															
	1 mean	CV -1	2 mean	CV -2	3 mean	CV-3	4 mean	CV -4	5 mean	CV -5	6 mean	CV -6	7 mean	CV -7	8 mean	CV -8
Sum of Betaine-Related Metabolites	9.72	7.86	6.37	19.04	7.83	13.07	7.68	13.47	9.39	15.05	6.49	18.16	6.46	11.05	10.36	14.65
Sum of Dimethylated Arg	1.89	10.63	0.85	36.13	1.6	21.06	1.21	22.02	1.94	20.91	1.32	20.97	1.51	13.96	2.1	13.38
Polyamine Synthesis	2.38	9.55	4.48	18.50	2.07	14.65	3.09	23.68	1.69	13.95	1.52	14.37	2.7	21.58	1.47	23.17
Putrescine Synthesis	0.41	26.71	1.3	21.16	0.72	19.64	1.18	36.85	0.59	19.85	0.51	14.72	0.81	17.88	0.52	33.65
Sum of Aminobutyric Acids	47.52	13.31	23.13	32.05	40.97	21.87	32.64	22.32	47.16	22.49	47	21.58	52.88	18.92	64.08	39.47
Sarcosine Synthesis from Choline	1.21	21.83	1.1	17.51	1.41	12.66	1.2	13.02	1.52	10.81	0.76	20.08	1.57	14.14	1.55	26.25
3-Met-His Synthesis	0.1	15.35	0.13	8.76	0.15	13.40	0.15	14.06	0.15	8.93	0.1	11.02	0.14	7.14	0.13	18.98
AABA Synthesis	0.13	18.33	0.3	15.73	0.25	15.89	0.33	11.08	0.24	6.88	0.12	13.11	0.42	12.41	0.29	21.22
Asymmetrical Arg Methylation	0.01	21.73	6.04	83.84	0.05	26.23	0.25	47.51	0.03	17.94	0	18.76	0.01	14.90	0.02	37.30
BABA Synthesis	0	.	0	80.83	0	0.00	0	17.32	0	173.21	0	86.60	0	0.00	0	173.21
CPS Deficiency (NBS)	2.68	9.42	3.81	15.59	5.41	30.46	4.19	25.71	6.51	17.68	1.69	9.27	3.12	8.39	4.91	26.83
Cystine Synthesis	0.03	57.39	0.01	36.63	0.01	51.29	0	31.08	0	39.66	0.05	31.91	0.01	46.29	0.01	68.25
DOPA Synthesis	0	32.73	0.01	19.17	0.01	32.38	0.01	33.24	0.01	14.37	0	0.00	0	23.59	0.01	29.36
GABR	0.22	18.82	0.09	74.39	0.18	25.44	0.08	32.86	0.16	28.55	0.74	16.36	0.73	10.12	0.5	36.37
HArg Synthesis	0	115.47	0.01	67.61	0	0.00	0	0.00	0	28.87	0	.	0	0.00	0	28.87
HCys Synthesis	0.08	17.21	0.36	26.38	0.24	26.99	0.29	31.56	0.28	14.99	0.06	13.37	0.25	8.06	0.31	42.43
Met Oxidation	0.05	21.46	0.12	24.30	0.1	26.05	0.1	13.92	0.08	11.94	0.08	13.09	0.21	26.96	0.08	22.94
NO-Synthase activity	3.87	17.15	19.67	33.60	12.47	27.18	53.04	37.21	7.84	24.84	1.67	18.04	2.4	10.19	4.11	41.30
Orn Synthesis	0.91	23.00	4.3	20.19	2.65	21.82	6.8	22.12	1.76	32.04	0.14	10.84	0.38	11.06	1.22	33.77
Ratio of Pro to Cit	0.73	8.40	1.33	18.53	0.93	7.47	1.28	13.65	0.78	17.11	0.63	14.02	1.16	4.00	1.05	11.86
Sarcosine Synthesis from Gly	0.05	26.76	0.11	19.81	0.08	22.45	0.13	25.33	0.08	9.23	0.04	16.55	0.1	6.60	0.08	24.76
Sum of Asym. and Sym. Arg Methylation	0.02	23.09	10.23	81.05	0.08	23.61	0.4	47.66	0.04	17.37	0	11.66	0.02	12.96	0.03	41.38
Symmetrical Arg Methylation	0.01	30.07	4.18	78.47	0.03	20.84	0.15	46.82	0.02	20.19	0	14.43	0.01	12.38	0.01	48.05
Taurine Synthesis	0.71	14.19	1.78	17.89	1.26	25.04	1.8	17.09	0.92	16.23	1.41	18.23	1.62	13.20	0.91	23.87
GABA Synthesis	0.01	29.49	0.03	45.37	0.01	18.05	0.03	34.53	0.01	14.68	0.01	22.69	0.01	5.43	0.01	22.17
Histamine Synthesis	0.05	27.16	0.19	17.76	0.13	24.37	0.17	20.97	0.13	15.72	0.07	17.97	0.11	13.69	0.11	27.20

Protocol Metabolite	[16]															
	1 mean	CV -1	2 mean	CV -2	3 mean	CV-3	4 mean	CV -4	5 mean	CV -5	6 mean	CV -6	7 mean	CV -7	8 mean	CV -8
PEA Synthesis	0	.	0	.	0	.	0	.	0	.	0	173.21	0	43.30	0	.
Serotonin Synthesis	0.02	21.17	0.32	60.79	0.08	23.58	0.16	49.68	1.54	65.78	0.02	12.12	0.05	11.49	0.06	22.35
p-Cresol-SO ₄ Synthesis	0.05	18.90	0.06	21.97	0.04	13.46	0.05	22.24	0.04	22.65	0.01	27.29	0.02	35.14	0.03	15.77
Indole Synthesis	24.67	26.20	173.87	66.90	44.21	20.18	76.38	44.54	619.93	66.06	7.48	13.56	18.74	10.16	40.23	30.44
7 α -Dehydroxylation of CA	7.47	20.75	10.89	40.03	9.39	24.99	8.13	54.63	11.62	48.75	7.11	25.14	7.89	42.62	10.52	46.86
GDCA Synthesis from CA	0.01	84.09	0.02	84.34	0.04	77.89	0.04	46.55	0.03	51.93	0.05	103.57	0.05	37.20	0.03	38.45
GLCA Synthesis from CDCA	0.03	73.17	0.01	75.29	0.01	90.03	0.01	70.62	0.01	61.42	0.01	82.92	0.01	81.31	0.01	75.41
Gly Conjugation of CA	0.06	36.07	0.06	67.16	0.19	54.31	0.35	74.64	0.16	51.92	0.11	42.65	0.15	28.26	0.53	60.24
Gly Conjugation of CDCA	0.32	77.45	0.13	86.83	0.24	73.16	0.21	58.34	0.15	55.75	0.21	77.57	0.6	58.45	0.37	60.16
Gly Conjugation of DCA	0	93.30	0	115.36	0.01	79.88	0	54.58	0	33.16	0.01	99.02	0.01	89.74	0	42.10
Gly Conjugation of Primary BAs	0.11	26.20	0.08	77.20	0.21	71.14	0.29	65.17	0.15	41.04	0.14	76.26	0.24	33.40	0.4	45.99
Primary BA Conjugation	0.18	29.29	0.22	64.47	0.36	68.53	0.52	55.65	0.3	36.07	0.17	74.37	0.42	24.96	0.69	38.87
Ratio of 12 α -OH BAs to Non-12 α -O	30.06	47.88	13.16	71.08	5.98	46.17	7.38	60.09	9.19	47.80	5.21	50.68	6.51	63.44	8.88	54.55
Ratio of CDCA to CA	0.21	43.38	0.95	62.75	1.31	50.76	1.26	46.50	1.03	41.17	1.59	62.33	1.17	39.68	1.08	30.08
Ratio of Primary BAs to BAs	0.28	15.48	0.27	45.62	0.34	25.57	0.33	35.00	0.31	27.93	0.35	31.47	0.34	47.21	0.31	30.99
Ratio of Secondary BAs to BAs	0.72	4.88	0.73	17.92	0.66	15.94	0.67	16.00	0.69	15.98	0.65	20.29	0.66	22.12	0.69	15.22
Secondary BA Conjugation	0.02	52.93	0.01	77.73	0.02	78.31	0.01	51.27	0.01	20.15	0.02	83.88	0.02	62.50	0.01	30.04
Secondary BA Synthesis	5.21	18.49	4.8	54.13	2.88	38.86	2.47	41.76	3.63	49.23	2.49	43.05	2.62	53.40	3.09	49.00
Sum of 12 α -OH BAs	31.83	32.70	90.76	30.21	106.92	37.22	93.29	20.68	118.06	26.97	100	35.31	100.51	29.10	120.8	29.44
Sum of BAs	33.27	32.53	107.38	27.46	138.98	50.73	113.44	21.29	132.71	28.94	138.58	49.26	126.26	43.04	135.76	31.73
Sum of Conjugated BAs	0.51	17.50	6.49	70.12	12.07	90.04	8.08	72.49	5.58	31.60	8.56	65.86	12.38	78.58	7.58	39.71
Sum of Conjugated Primary BAs	0.41	23.76	5.47	71.21	10	90.74	6.74	74.07	4.82	32.40	6.73	67.64	10.2	77.70	6.77	41.83
Sum of Conjugated Secondary BAs	0.1	28.37	1.02	61.54	2.08	83.77	1.35	47.68	0.76	24.93	1.83	72.36	2.18	77.32	0.81	28.57
Sum of Gly-Conjugated BAs	0.22	24.10	2.18	79.81	4.48	90.21	2.9	63.95	2.2	30.30	5.31	64.91	5.52	83.46	3.31	40.04
Sum of Non-12 α -OH BAs	1.44	37.61	16.67	71.71	32.44	88.82	20.2	72.83	14.59	59.18	38.53	87.77	25.84	93.01	14.97	56.76
Sum of Primary BAs	11.97	32.68	33.45	47.64	56.76	72.72	38.14	51.70	38.05	50.38	63.15	73.63	48.11	84.63	36.75	46.96

Protocol Metabolite	[17]															
	1 mean	CV -1	2 mean	CV -2	3 mean	CV-3	4 mean	CV -4	5 mean	CV -5	6 mean	CV -6	7 mean	CV -7	8 mean	CV -8
Sum of Secondary BAs	21.29	33.23	73.92	31.92	82.53	33.67	75.32	20.51	94.77	18.92	75.24	31.18	78.33	23.20	99.13	31.17
Sum of Taurine-Conjugated BAs	0.28	22.27	4.31	75.50	7.59	91.54	5.18	78.81	3.38	34.18	3.24	73.46	6.87	79.60	4.28	38.32
Sum of Unconjugated BAs	32.75	33.79	100.9	27.03	127.23	47.57	105.17	20.52	127.02	30.57	129.79	48.29	114.06	37.40	128.17	38.66
Sum of Unconjugated Primary BAs	11.55	35.64	28	46.34	46.74	73.23	31.4	65.20	33.22	56.38	56.41	76.81	37.86	87.49	29.96	63.24
Taurine Conjugation of CA	0.06	40.59	0.1	45.17	0.15	66.18	0.27	58.06	0.18	42.26	0.02	78.65	0.19	17.56	0.38	38.12
Taurine Conjugation of CDCA	0.12	78.06	0.19	81.77	0.16	62.17	0.2	64.17	0.17	49.51	0.03	91.48	0.29	55.47	0.27	52.63
Taurine Conjugation of DCA	0	50.69	0.01	113.71	0.01	86.34	0.01	85.69	0	33.79	0.01	107.77	0.01	76.08	0	37.53
Taurine Conjugation of Primary BAs	0.07	29.74	0.13	56.50	0.15	66.60	0.23	55.90	0.15	35.16	0.02	83.89	0.19	25.02	0.29	38.92
TDCA Synthesis from CA	0.01	48.64	0.03	71.30	0.04	83.71	0.04	60.29	0.03	35.84	0.01	100.86	0.04	30.59	0.04	35.99
TLCA Synthesis from CDCA	0.02	62.89	0.02	62.70	0.02	46.93	0.01	46.18	0.02	61.46	0	96.64	0.03	77.32	0.02	67.94
Spermidine Synthesis	4.68	24.15	2.25	24.51	1.69	24.95	1.5	26.70	1.72	30.64	1.8	12.10	2.54	26.57	1.78	37.10
Spermine Synthesis	0.02	9.60	0.04	17.60	0.04	18.30	0.08	29.27	0.04	29.69	0.03	20.85	0.05	18.24	0.04	12.67
Sum of Neurotransmitters	6.24	10.70	6.49	14.70	7.4	14.03	7.06	12.73	8.82	10.95	6.18	13.77	6.27	13.30	8.47	13.71
Sum of Polyamines	199.56	5.13	58.1	31.32	68.34	21.40	44.97	39.59	80.78	23.51	62.32	21.03	37.64	24.73	73.2	21.47
Ratio of DHA to arachidonic acid	0.69	26.43	0.53	11.47	0.56	11.76	0.6	17.70	0.62	12.82	0.52	9.31	0.58	13.54	0.54	13.33
Ratio of DHA to EPA	2.21	31.06	4.27	10.10	3.71	29.28	3.91	14.65	4	8.24	3.82	13.11	4.26	21.92	3.49	21.32
Ratio of EPA to arachidonic acid	0.39	22.08	0.14	15.12	0.2	30.40	0.19	13.45	0.2	17.60	0.17	12.76	0.2	26.68	0.2	13.66
Sum of Measured w-3 FAs	0.25	20.11	8.21	19.23	11.32	35.24	9.47	18.14	9.57	27.41	11.9	20.25	11.34	26.89	8.92	20.36
Sum of MUFAs	179.16	43.11	2080.67	26.42	1697.11	29.51	1481.67	23.19	1766.89	16.55	5813.11	40.26	5792.33	24.94	1563.56	15.12
Sum of PUFAs	341.11	38.78	1533.78	20.63	2147	27.35	1777.44	20.80	1895.78	8.77	2807.44	32.64	2415.67	25.17	1801.33	19.65
PLA2 Activity (2)	8.17	46.50	27.39	42.28	142.43	60.89	32.93	41.94	61.59	50.46	87.08	67.54	20.84	39.96	36.36	28.82
PLA2 Activity (4)	4.4	138.70	72.94	31.67	177.34	26.31	116.2	28.95	146	.	210.27	79.13	71.65	76.30	55.85	71.11
PLA2 Activity (6)	6.05	44.53	85.9	17.34	259.58	31.71	169.8	49.95	387.53	68.22	269.38	56.60	98.99	26.20	115.7	39.78
3-IAA Synthesis	0.05	8.82	0.04	11.49	0.05	15.80	0.04	12.75	0.05	12.24	0.05	15.55	0.08	8.96	0.05	16.16
3-IPA Synthesis	0.02	18.11	0.01	12.53	0.02	22.37	0.01	14.99	0.02	10.19	0.02	18.25	0.03	11.82	0.01	23.73
Sum of Purines	571.89	10.66	230.78	27.56	421.67	15.93	360.56	34.65	303.67	23.48	638.11	25.30	267.78	15.32	386.96	32.54
Xanthine Synthesis	1.33	38.72	1.3	44.51	1.29	40.96	1.63	40.51	1.45	13.85	0.8	30.95	2.11	7.37	1.78	30.70

[18]

Concentrations below the LOD are marked in grey.

Abbreviations: 12a-OH BAs, 12-alpha hydroxylated bile acids, 3-IAA, 3-indoleacetic acid; 3-IPA, 3-indolepropionic acid; AA, amino acid; AABA, alpha-aminobutyric acid; ADMA, asymmetric dimethylarginine; Asn, asparagine; BA, bile acid; BABA, beta-aminobutyric acid; CA, cholic acid; CACT, carnitine-acylcarnitine translocase; CDCA, chenodeoxycholic acid; Cit, citrulline; CPS, carbamoyl phosphate synthetase; CPT1, carnitine palmitoyltransferase 1; Cys, cysteine; DCA, deoxycholic acid; DHA, docosahexaenoic acid; DLD, dihydrolipoamide dehydrogenase; DOPA, dihydroxyphenylalanine; EPA, eicosapentaenoic acid; FA, fatty acid; HipAcid, hippuric acid; GABA, gamma-aminobutyric acid; GABR, global arginine bioavailability ratio; Gly, glycine; GSH, glutathione; HArg, homoarginine; HCys, homocysteine; His, histidine; Met, methionine; MTHFR, methylene tetrahydrofolate reductase; MUFA, mono unsaturated fatty acid; NBS, newborn screening; NO, nitric oxide; Orn, ornithine; OTC, ornithine transcarbamylase; p-cresol SO₄, p-cresol sulfate; PEA, phenylethylamine; PKU, phenylketonuria; PLA2, phospholipase 2; Pro, proline; PUFA, poly unsaturated fatty acid; SDMA, symmetric dimethylarginine; TDCA, taurodeoxycholic acid; TLCA, tauroolithocholic acid; TMAO, trimethylamine N-oxide.

[19]

Supplementary Table 3. Distribution of mean intra-individual coefficients of variation (CV) for individual metabolites by stool preparation protocol

CV range	Protocol 1 n [%]	Protocol 2 n [%]	Protocol 3 n [%]	Protocol 4 n [%]	Protocol 5 n [%]	Protocol 6 n [%]	Protocol 7 n [%]	Protocol 8 n [%]
0-15%	34 (11.5)	16 (4.4)	21 (7.2)	22 (7.0)	20 (6.4)	19 (5.2)	33 (9.1)	21 (6.4)
15-30%	60 (20.3)	70 (19.3)	67 (23.0)	67 (21.3)	88 (28.2)	89 (24.5)	70 (19.3)	61 (18.5)
30-40%	16 (5.4)	51 (14.1)	19 (6.5)	18 (5.7)	17 (5.4)	46 (12.7)	22 (6.1)	31 (9.4)
40-50%	7 (2.4)	32 (8.8)	16 (5.5)	17 (5.4)	8 (2.6)	34 (9.4)	38 (10.5)	15 (4.5)
50-60%	9 (3.0)	25 (6.9)	10 (3.4)	21 (6.7)	9 (2.9)	25 (6.9)	19 (5.2)	13 (3.9)
60-70%	15 (5.1)	28 (7.7)	11 (3.8)	21 (6.7)	12 (3.8)	26 (7.2)	22 (6.1)	15 (4.5)
70-80%	8 (2.7)	30 (8.3)	7 (2.4)	8 (2.5)	12 (3.8)	20 (5.5)	32 (8.8)	14 (4.2)
80-90%	15 (5.1)	27 (7.5)	12 (4.1)	14 (4.4)	18 (5.8)	13 (3.6)	22 (6.1)	15 (4.5)
90-100%	13 (4.4)	20 (5.5)	24 (8.2)	26 (8.3)	18 (5.8)	27 (7.4)	34 (9.4)	14 (4.2)
>100%	119 (40.2)	63 (17.4)	104 (35.7)	101 (32.1)	110 (35.3)	64 (17.6)	71 (19.6)	131 (39.7)

The distributions are shown as absolute numbers and percentages for each specified CV range.