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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	1		2		3		4		5		6		7		8	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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, Acetylornithine; ADMA, Asymmetric dimethylarginine; Ala, Alanine; alpha-AAA, alpha Aminoadipic acid; Arg, Arginine; Asn, asparagine; Asp, aspartate; BABA, beta-Aminobutyric acid; betaAla, beta-Alanine; C0, Carnitine; C7-DC, Pimeloylcarnitine; C8, Octanoylcarnitine; C9, Nonaylcarnitine; 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), Octdecadienoic 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 aicd; 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, Taurolithocholic acid; TMAO, Trimethylamine N-oxide; TMCA, Tauromurocholic 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	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**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

[15]

Protocol	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**mean**	**CV -1**	**mean**	**CV -2**	**mean**	**CV-3**	**mean**	**CV -4**	**mean**	**CV -5**	**mean**	**CV -6**	**mean**	**CV -7**	**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

[16]

Protocol	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**mean**	**CV -1**	**mean**	**CV -2**	**mean**	**CV-3**	**mean**	**CV -4**	**mean**	**CV -5**	**mean**	**CV -6**	**mean**	**CV -7**	**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-SO4 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
7a-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 12a-OH BAs to Non-12a-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 12a-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-12a-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

[17]

Protocol	**1**		**2**		**3**		**4**		**5**		**6**		**7**		**8**	
Metabolite	**mean**	**CV -1**	**mean**	**CV -2**	**mean**	**CV-3**	**mean**	**CV -4**	**mean**	**CV -5**	**mean**	**CV -6**	**mean**	**CV -7**	**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

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 trancarbamylase; 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, taurolithocholic 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.