Supporting Information

A complementary method with PFBBr-derivatization based on GC-EI-MS platform for the simultaneous quantitation of short-, medium- and long -chain fatty acids in murine plasma and feces samples

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Table S1 The inter and intra-day of precision, accuracy for assays.

No.	Abbreviation	Inter-day assay (n=6)								Intra-day assay (n=18)							
		Precision (RSD%)				Accuracy (RE%)				Precision (RSD%)				Accuracy (RE%)			
		LLOQ	QCL	QCM	QCH	LLOQ	QCL	QCM	QCH	LLOQ	QCL	QCM	QCH	LLOQ	QCL	QCM	QCH
1	FA 2:0	1.42	0.78	2.61	0.89	106.55	99.67	95.70	90.73	4.39	6.79	3.23	4.16	109.86	103.33	101.73	94.04
2	FA 3:0	0.83	1.22	3.19	0.37	105.02	105.02	94.63	88.92	4.99	5.57	5.85	4.56	115.01	110.63	96.34	90.86
3	FA 4:1	1.03	1.16	3.47	0.50	108.61	99.05	94.28	91.69	5.39	5.47	7.51	5.42	117.03	111.16	93.76	92.28
4	FA 4:0	1.52	0.76	2.61	0.68	106.49	97.49	87.63	86.36	5.73	5.18	5.55	5.89	107.50	114.01	89.37	86.98
5	FA 5:1	2.53	3.80	3.37	0.56	115.53	105.53	94.41	93.43	4.91	11.52	7.02	3.91	116.78	114.22	94.65	96.49
6	FA 5:0	4.23	6.03	3.98	1.91	103.65	103.64	101.03	93.00	5.57	10.57	6.82	4.87	106.58	106.58	101.44	95.37
7	FA 6:0	2.37	1.51	9.08	1.21	112.50	102.51	86.07	91.60	17.07	5.69	13.23	5.70	117.37	110.13	88.32	92.44
8	FA 7:0	5.56	10.37	7.82	1.43	112.95	107.95	89.93	90.54	14.63	12.63	13.85	6.15	117.85	110.11	85.99	90.93
9	FA 8:0	5.99	7.71	7.29	0.93	103.69	113.69	107.66	111.72	11.88	13.54	11.53	4.24	111.59	101.59	114.75	112.74
10	FA 9:0	10.58	11.29	6.48	2.67	89.84	99.84	86.53	103.62	13.37	10.41	9.13	8.24	101.30	101.30	93.06	110.85
11	FA 10:0	6.74	0.91	1.61	1.76	100.34	109.74	110.13	113.11	7.95	8.91	11.69	4.96	114.14	102.14	113.45	113.36
12	FA 11:0	13.58	2.21	1.62	4.39	109.02	89.01	96.81	106.71	13.92	10.51	13.42	11.36	115.53	95.53	92.79	110.42
13	FA 12:0	11.32	1.33	11.96	2.56	109.47	99.47	87.49	104.52	14.81	14.07	14.73	11.81	112.35	92.35	85.51	106.89
14	FA 13:0	15.48	14.86	6.29	7.21	108.40	88.40	88.08	101.90	17.25	11.14	14.39	10.25	116.17	106.17	90.68	102.60
15	FA 14:1	14.58	2.48	0.79	8.72	109.16	90.17	95.37	92.44	16.99	5.25	7.58	18.85	110.37	114.38	104.09	90.59
16	FA 14:0	7.87	6.14	12.87	7.59	104.93	89.31	97.26	110.37	12.26	13.79	10.78	14.41	85.94	98.51	114.64	112.70
17	FA 15:1	9.90	3.68	8.76	8.06	99.33	93.31	90.57	85.18	17.82	14.25	10.64	14.86	118.69	98.71	87.03	89.05
18	FA 15:0	15.63	4.89	1.75	7.76	118.32	110.33	85.36	102.67	17.81	13.11	8.56	14.14	88.94	93.41	92.30	102.53
19	FA 16:1T	10.64	9.33	2.08	7.73	108.36	95.76	105.10	92.25	13.69	13.78	6.70	10.29	95.63	112.69	113.91	92.31
20	FA 16:1	5.03	10.79	3.07	7.80	116.35	109.47	97.67	95.91	19.55	10.92	8.49	10.36	117.63	112.59	108.11	95.52
21	FA 16:0	4.38	12.75	9.33	4.02	83.36	89.23	98.89	106.18	9.16	7.60	11.29	10.54	82.93	86.46	88.60	111.34
22	FA 17:1T	10.66	5.01	0.42	5.59	95.36	89.15	113.23	95.71	12.56	12.60	5.12	13.08	99.88	97.62	108.88	96.83

23	FA 17:0	11.04	3.41	4.14	7.19	102.33	88.12	112.31	98.85	13.25	7.69	6.24	10.41	102.44	110.88	110.85	98.82
24	FA 18:3N6	12.90	8.02	2.47	3.78	103.65	99.59	104.29	89.96	16.30	14.61	14.03	6.31	118.43	111.99	114.44	87.68
25	FA 18:2N6	13.84	13.08	1.74	4.14	112.38	102.51	86.39	89.61	15.61	12.79	6.16	8.53	112.56	108.95	85.26	86.85
26	FA 18:1N9C	4.30	3.51	1.92	5.90	89.36	88.25	87.03	89.62	9.77	11.63	5.44	12.84	110.89	96.32	85.23	85.16
27	FA 18:3N3	12.62	9.38	2.35	5.60	116.29	114.22	86.48	86.66	15.33	11.17	10.78	11.01	109.68	114.32	86.42	90.98
28	FA 18:1N9T	10.18	9.16	2.88	6.48	109.94	105.69	99.49	87.06	18.15	12.07	11.26	12.23	99.59	96.59	94.07	93.80
29	FA 18:1N7	11.88	9.43	2.86	5.48	118.49	110.06	114.95	89.38	14.51	13.26	8.17	12.67	107.59	95.33	113.43	85.28
30	FA 18:0	8.63	13.04	11.27	6.43	109.58	88.69	112.48	105.85	9.88	10.40	12.44	13.84	110.39	96.32	112.96	109.79
31	FA 19:1N9T	13.64	6.67	2.19	3.91	106.89	112.63	102.27	88.25	17.71	9.57	3.73	8.37	110.95	112.17	102.89	89.61
32	FA 19:0	10.45	6.11	1.32	4.69	116.69	95.03	103.56	86.65	14.52	7.32	4.80	10.66	89.65	110.87	102.30	86.06
33	FA 20:4N6	11.53	10.29	4.35	3.04	112.45	96.25	102.39	86.71	13.93	14.43	5.61	4.05	109.75	103.86	102.70	87.09
34	FA 20:5N3	9.87	10.98	5.91	5.25	104.75	92.51	89.17	89.14	14.25	10.47	7.78	3.75	100.85	90.25	86.15	91.18
35	FA 20:1T	10.07	12.31	9.44	3.46	112.59	105.57	111.59	93.13	12.91	14.47	10.44	7.06	109.59	114.18	114.32	91.88
36	FA 20:1	8.09	12.71	7.67	4.05	116.35	90.23	114.59	88.19	13.95	14.39	10.52	8.38	115.84	95.11	112.93	85.79
37	FA 20:2	10.34	13.35	4.27	5.76	98.56	105.05	107.85	87.66	11.50	14.11	9.56	9.49	102.59	114.94	108.68	85.06
38	FA 20:0	9.01	1.79	3.49	5.40	94.55	101.84	95.91	91.54	10.16	7.10	6.16	12.26	112.86	110.57	93.73	87.09
39	FA 21:0	5.89	5.00	2.93	3.44	108.55	98.45	109.58	86.61	8.74	7.59	13.75	8.39	109.63	93.46	106.03	87.70
40	FA 22:0	14.61	12.69	9.92	13.32	81.29	95.82	110.14	97.31	19.30	12.00	13.99	13.01	107.59	94.25	100.18	98.02
41	FA 22:6N3	12.29	11.21	3.96	1.82	80.99	112.81	95.23	87.12	16.89	11.06	7.07	4.74	100.29	94.22	104.76	86.42
42	FA 22:2	10.91	5.89	0.82	3.33	109.28	104.32	98.99	87.96	11.80	6.50	3.97	8.42	114.87	112.63	98.87	86.18
43	FA 23:0	9.05	6.71	2.24	3.25	99.57	104.09	101.48	88.23	9.96	9.08	4.74	8.23	118.52	110.58	100.68	88.71
44	FA 24:0	10.52	6.05	2.16	2.32	96.59	101.89	93.03	86.74	12.73	5.41	3.18	7.39	110.35	100.15	94.06	89.76

Table S2. The matrix effect, extraction recovery and stability for assays.

NO.	Abbreviation	Extraction recovery (%)			Matrix effect (%)			Stability (%)	
		QCL	QCM	QCH	QCL	QCM	QCH	24 h	48 h
1	FA 2:0	89.53	118.79	117.73	89.63	86.46	87.25	92.48	92.64
2	FA 3:0	86.14	117.49	88.00	86.97	85.44	89.22	91.68	92.11
3	FA 4:1	83.19	94.82	109.12	85.63	91.80	99.01	90.26	90.80
4	FA 4:0	89.01	87.10	103.58	86.51	88.09	94.52	89.34	89.74
5	FA 5:1	100.41	101.79	108.25	102.78	97.81	98.21	93.72	94.26
6	FA 5:0	85.56	87.41	108.01	88.12	86.82	97.91	93.06	93.82
7	FA 6:0	83.42	104.42	111.56	90.02	101.93	101.36	92.08	93.16
8	FA 7:0	89.03	103.93	112.37	89.30	100.44	101.99	91.88	92.98
9	FA 8:0	81.41	104.96	108.42	85.98	88.81	86.55	93.71	94.40
10	FA 9:0	85.08	104.16	116.12	88.98	88.01	92.77	89.45	91.32
11	FA 10:0	94.66	115.81	109.47	110.48	99.08	87.57	93.13	93.85
12	FA 11:0	98.98	115.29	120.71	100.34	104.59	98.06	86.67	89.34
13	FA 12:0	88.21	106.13	114.81	86.32	89.86	99.62	84.65	87.56
14	FA 13:0	88.27	120.39	119.25	91.17	101.44	104.50	82.41	85.88
15	FA 14:1	92.61	108.29	117.36	95.53	107.60	114.11	77.26	81.57
16	FA 14:0	96.20	86.53	118.02	87.09	90.35	105.12	84.96	87.82
17	FA 15:1	105.21	110.58	118.69	113.66	114.89	110.90	73.11	77.00
18	FA 15:0	100.15	103.06	113.95	105.50	114.34	113.44	80.19	84.00
19	FA 16:1T	79.09	116.84	117.01	102.29	112.35	103.61	80.51	83.08
20	FA 16:1	103.45	107.50	116.55	92.44	97.31	110.60	79.24	83.45
21	FA 16:0	93.28	102.97	114.98	117.14	111.73	108.38	86.48	88.84
22	FA 17:1T	83.83	106.38	97.85	86.24	89.83	113.42	81.30	84.03
23	FA 17:0	100.57	120.23	153.62	112.23	113.44	104.83	79.90	83.38

24	FA 18:3N6	96.43	97.13	118.13	91.07	89.96	112.23	90.67	93.49
25	FA 18:2N6	110.72	117.27	118.16	105.48	103.11	108.36	87.34	88.65
26	FA 18:1N9C	88.32	112.17	119.53	108.73	107.12	112.91	81.64	84.01
27	FA 18:3N3	101.35	109.29	112.15	104.82	106.57	100.45	87.37	89.37
28	FA 18:1N9T	110.92	115.26	118.64	98.14	86.42	100.14	83.07	85.79
29	FA 18:1N7	108.90	104.85	117.55	103.36	86.25	112.25	83.12	85.93
30	FA 18:0	97.58	83.85	116.84	99.37	90.30	107.22	80.42	83.95
31	FA 19:1N9T	108.78	77.35	117.46	103.17	85.19	112.88	87.63	89.27
32	FA 19:0	106.40	110.91	119.58	110.35	110.23	102.61	84.33	86.20
33	FA 20:4N6	104.03	107.26	113.31	102.77	110.96	114.34	92.77	93.35
34	FA 20:5N3	87.05	107.80	112.61	119.55	113.28	112.89	98.00	89.99
35	FA 20:1T	105.03	96.00	113.45	104.58	106.40	113.18	92.01	93.53
36	FA 20:1	81.35	110.11	117.86	113.39	104.11	109.21	88.46	89.59
37	FA 20:2	91.96	88.95	116.80	89.43	108.29	111.60	88.92	87.94
38	FA 20:0	113.30	103.61	114.95	110.81	112.52	113.22	83.67	85.81
39	FA 21:0	88.24	90.58	113.13	89.37	82.58	102.18	86.94	88.08
40	FA 22:0	107.22	117.47	119.23	88.31	113.57	111.78	95.13	95.17
41	FA 22:6N3	80.32	91.08	108.73	103.25	109.85	114.21	93.45	93.39
42	FA 22:2	109.18	108.45	115.82	106.52	111.06	107.09	87.04	88.36
43	FA 23:0	104.97	114.50	112.60	102.09	106.69	103.67	87.03	88.34
44	FA 24:0	113.36	114.41	111.67	113.28	107.39	102.63	88.70	89.11

Table S3. The changes of FAs levels in different groups in feces and plasma

No.	Abbreviation	Control group (mean ± SD)	DON group (mean ± SD)	Control group versus DON group		
				VIP value[a]	*p*-value[b]	Fold change
1	FA 2:0_F	83.21±46.67	141.30±51.86	0.8353	0.0260	0.59
2	FA 4:1_F	1.80±1.19	0.95±0.48	0.8729	0.0485	1.89
3	FA 4:0_F	6.79±5.84	17.26±9.41	0.8011	0.0062	0.39
4	FA 10:0_F	3.53±2.07	11.14±4.18	1.1898	0.0005	0.32
5	FA 14:0_F	2.75±0.62	8.66±2.24	1.5209	＜0.0001	0.32
6	FA 15:0_F	3.96±1.63	10.93±3.61	0.4692	＜0.0001	0.36
7	FA 16:1T_F	1.72±0.41	3.12±0.81	1.3185	0.0004	0.55
8	FA 16:0_F	71.68±20.05	171.60±32.69	1.4937	＜0.0001	0.42
9	FA 17:0_F	3.36±0.72	7.63±0.73	1.5963	＜0.0001	0.44
10	FA 18:1N9C_F	27.78±10.93	57.83±16.18	1.3110	0.0003	0.48
11	FA 18:1N9T_F	4.23±1.37	11.26±4.62	1.3051	0.0004	0.38
12	FA 18:0_F	73.10±12.98	129.43±15.09	1.5023	＜0.0001	0.56
13	FA 19:0_F	1.65±0.38	2.31±0.32	1.1276	0.0010	0.71
14	FA 20:0_F	18.00±4.51	21.64±2.75	0.7521	0.0569	0.83
15	FA 23:0_F	6.07±1.64	8.76±0.87	1.1864	0.0002	0.69
16	FA 10:0_P	36.24±16.61	51.17±11.21	1.4051	0.0211	0.71
17	FA 12:0_P	11.50±10.39	18.64±9.50	1.0834	0.0894	0.62
18	FA 14:1_P	0.89±0.23	0.69±0.19	1.2145	0.0836	1.29
19	FA 16:1_P	1.81±2.08	0.25±0.36	1.4599	0.0301	7.34
20	FA 17:0_P	0.16±0.05	0.23±0.10	1.3034	0.0340	0.67
21	FA 20:4N6_P	2.89±0.75	2.02±0.55	1.5857	0.0095	1.43

a The VIP value was from the OPLS mode.

b The *p*-value was calculated from the Student's *t*-test.