



Supplementary Information

A Chemometric Model Applied to Fatty Acid Determination in Blood

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Table S1. Retention time and relative abundance of the ions with *m/z* 74, 79, 81 and 87 in mass spectra obtained by SIM for individual FAME

FAME	<i>t_r</i> ± SD ^b	Relative abundance of fragments in MS-SIM, mean ± SD ^a / %			
		<i>m/z</i> 74	<i>m/z</i> 79	<i>m/z</i> 81	<i>m/z</i> 87
10:0 ^c	5.563 ± 0.00	100	0.63 ± 0.05	1.45 ± 0.28	54.64 ± 1.17
11:0 ^c	7.377 ± 0.05	100	0.61 ± 0.28	1.80 ± 0.95	58.21 ± 0.71
12:0	8.458 ± 0.08	100	0.77 ± 0.05	1.52 ± 0.22	62.27 ± 1.15
13:0	8.690 ± 0.08	100	0.89 ± 0.07	3.19 ± 3.66	64.44 ± 0.80
14:1	9.949 ± 0.04	100	15.34 ± 0.69	42.06 ± 10.04	72.43 ± 0.75
14:0	10.122 ± 0.04	100	0.91 ± 0.04	2.46 ± 1.24	67.31 ± 1.14
15:1	11.783 ± 0.03	100	14.89 ± 0.69	41.78 ± 13.74	73.16 ± 0.65
15:0	11.993 ± 0.03	100	0.96 ± 0.07	3.52 ± 3.48	68.53 ± 0.57
16:1	13.718 ± 0.03	100	17.48 ± 0.80	50.38 ± 6.2	73.31 ± 0.74
16:0	14.156 ± 0.02	100	0.95 ± 0.02	2.58 ± 0.48	70.71 ± 1.22
17:1	16.068 ± 0.03	100	16.74 ± 0.71	46.54 ± 15.21	73.66 ± 0.82
17:0	16.552 ± 0.02	100	1.02 ± 0.05	5.01 ± 6.10	71.30 ± 0.55
18:3n6	17.908 ± 0.02	11.72 ± 0.19	100	58.20 ± 1.49	18.78 ± 0.80
18:2n6	18.298 ± 0.02	12.80 ± 3.17	43.85 ± 10.91	100	9.27 ± 2.29
18:3n3 ^d	18.573 ± 0.02	10.37 ± 1.48	100	63.85 ± 1.22	20.38 ± 1.12
18:1 ^d	18.573 ± 0.02	100	23.07 ± 1.79	59.81 ± 15.22	75.95 ± 0.71
18:0	18.603 ± 0.02	100	1.04 ± 0.03	3.06 ± 0.49	72.83 ± 0.87
19:0 ^e	20.896 ± 0.02	100	1.02 ± 0.03	3.20 ± 0.38	74.38 ± 0.69
20:4n6	22.525 ± 0.02	16.13 ± 0.60	100	37.17 ± 2.42	8.20 ± 0.26
20:5n3	22.695 ± 0.02	12.13 ± 0.49	100	30.18 ± 13.25	6.04 ± 0.17
20:3n6	22.769 ± 0.02	12.65 ± 0.48	100	71.57 ± 0.76	20.43 ± 0.54
20:2n6	23.071 ± 0.02	18.02 ± 1.00	42.70 ± 1.36	100	10.87 ± 0.29
20:1	23.507 ± 0.13	100	18.06 ± 0.38	60.26 ± 0.83	72.86 ± 1.79
20:0	24.377 ± 0.02	100	1.09 ± 0.02	3.08 ± 0.64	75.21 ± 0.85
21:0	27.014 ± 0.02	100	0.77 ± 0.53	4.00 ± 1.08	76.15 ± 0.45
22:6n3	27.626 ± 0.00	1.22 ± 0.65	100	20.24 ± 0.32	2.69 ± 2.11
22:2n6	28.828 ± 0.00	23.11 ± 1.53	39.89 ± 1.22	100	12.65 ± 1.11
22:1	28.924 ± 0.04	100	17.83 ± 0.37	55.60 ± 13.53	72.78 ± 1.15
22:0	29.614 ± 0.03	100	1.10 ± 0.02	3.55 ± 0.80	77.64 ± 0.90
23:0	32.156 ± 0.04	100	0.79 ± 0.54	5.24 ± 2.99	78.61 ± 0.52
24:1	32.842 ± 0.06	100	13.04 ± 0.39	50.61 ± 5.89	69.57 ± 1.77
24:0	33.756 ± 0.03	100	1.15 ± 0.04	3.80 ± 1.53	80.05 ± 0.93

^aMean ± SD of seven injections; ^bchromatogram obtained as described in material and methods; ^c*p* < 0.05 compared with relative abundance of 0 class (saturated); ^davailable as individual standard; ^einternal standard; *t_r*, retention time.

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Table S2. Relative abundance of the ions with m/z 74, 79, 81 and 87 in mass spectra obtained by SIM for contaminations, artifacts and co-elution

	Relative abundance of fragments in MS-SIM, mean \pm SD ^a / %			
	m/z 74	m/z 79	m/z 81	m/z 87
Decanol ^b	3.45 ^{e,f,g,h,i} \pm 0.19	28.69 ^{e,f,g,h,i} \pm 0.35	100 ^{e,f,h,i}	7.37 ^{e,f,h} \pm 0.94
Dodecanal	0.33 ^{e,f,g,h,i} \pm 0.15	18.83 ^{e,f,g,h,i} \pm 1.00	100 ^{e,f,h,i}	1.53 ^{e,f,g,h} \pm 0.21
Pentacosane	0.51 ^{e,f,g,h,i} \pm 0.24	32.46 ^{e,f,g,h,i} \pm 2.56	100 ^{e,f,h,i}	6.47 ^{e,f,h} \pm 0.45
20:1 + 20:3n3 ^c	15.59 ^{e,f,h,i} \pm 0.31	100 ^{e,f,g}	38.45 ^{e,f,h,i} \pm 0.46	8.02 ^{e,f,h} \pm 0.14

^aMean \pm SD of triplicate analyses; ^bchromatogram obtained as described in material and methods; ^cco-eluted FAME; ^e $p < 0.05$ compared with 0 class; ^f $p < 0.05$ compared with 1 class; ^g $p < 0.05$ compared with 2 class; ^h $p < 0.05$ compared with 3 class; ⁱ $p < 0.05$ compared with ≥ 4 class.

Table S3. Relative abundance of the ions with m/z 74, 79, 81 and 87 in mass spectra obtained by SIM from FA present in blood lipids

FAME	Relative abundance of fragments in MS-SIM, mean \pm SD ^a / %			
	m/z 74	m/z 79	m/z 81	m/z 87
14:0	100	0.77 \pm 0.64	1.82 \pm 0.84	65.76 \pm 2.52
15:0	100	0.00	1.43 \pm 1.79	73.94 \pm 4.34
16:1	100	14.15 \pm 2.99	52.53 \pm 6.77	72.89 \pm 6.34
16:0	100	0.83 \pm 0.37	2.13 \pm 0.94	74.59 \pm 2.14
17:1	100	15.42 \pm 7.79	54.58 \pm 13.73	73.88 \pm 8.48
17:0	100	0.32 \pm 0.54	2.40 \pm 1.15	70.89 \pm 2.17
18:3n6	8.98 \pm 4.55	100	55.59 \pm 5.70	19.86 \pm 1.60
18:2n6	11.32 \pm 3.63	44.95 \pm 1.18	100	8.95 \pm 1.62
18:1	100	23.22 \pm 2.61	58.72 \pm 8.16	73.68 \pm 8.42
18:0	100	0.65 \pm 0.44	1.87 \pm 1.31	74.67 \pm 3.76
19:0 ^b	100	0.97 \pm 0.08	2.99 \pm 0.27	77.53 \pm 2.85
20:4n6	15.02 \pm 0.92	100	35.79 \pm 2.76	7.69 \pm 0.31
20:5n3	12.43 \pm 0.68	100	31.46 \pm 2.66	7.23 \pm 2.12
20:3n6	11.34 \pm 0.73	100	71.50 \pm 6.41	19.97 \pm 1.16
20:2n6	17.34 \pm 1.43	44.67 \pm 6.17	100	9.35 \pm 2.76
20:0	100	1.38 \pm 1.61	2.60 \pm 1.89	77.51 \pm 4.38
22:6n3	1.64 \pm 1.36	100.00 \pm 0.00	20.82 \pm 3.03	1.88 \pm 0.92
22:0	100	0.72 \pm 0.74	4.05 \pm 2.20	77.29 \pm 1.66
24:1	100	10.59 \pm 4.08	46.51 \pm 14.15	65.27 \pm 3.93
24:0	100	1.56 \pm 3.42	3.36 \pm 1.66	79.45 \pm 4.54

^aValues are mean \pm SD (n = 8); ^binternal standard.

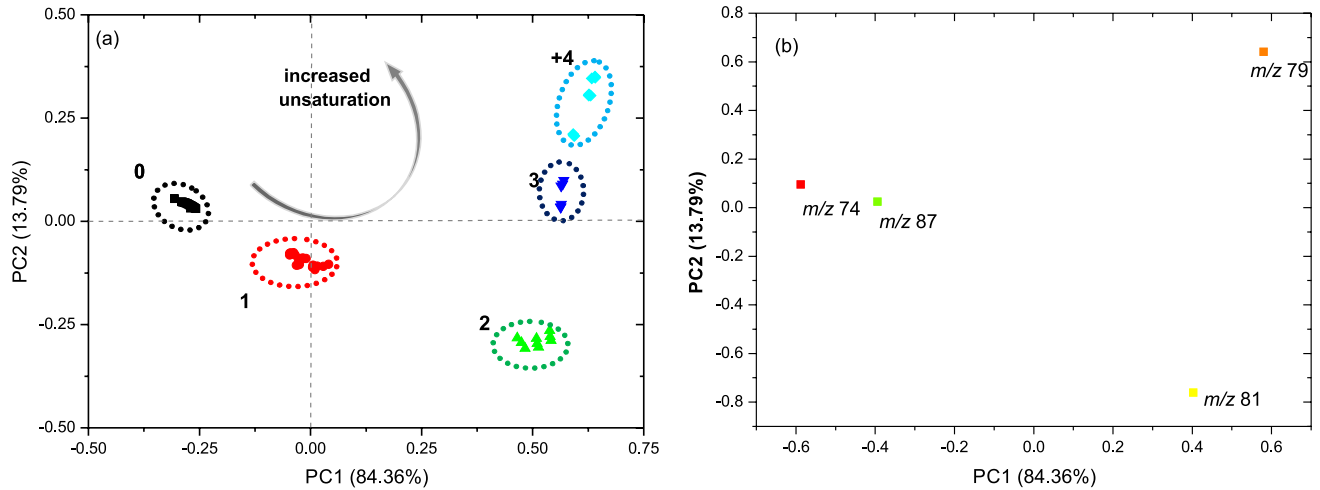


Figure S1. (a) Scores plot from PCA based on mass spectra in SIM mode (m/z 74, 79, 81 and 87), confirming the cluster of several FAME in five classes, according to the alkyl chain double bond number and (b) Loading plot highlighting the most important ions of the mass spectra. Legend: FAME class: 0, saturated (■); 1, one double bond (●); 2, two double bonds (▲); 3, three double bonds (▼); ≥ 4 , four, five or six double bonds (◆).

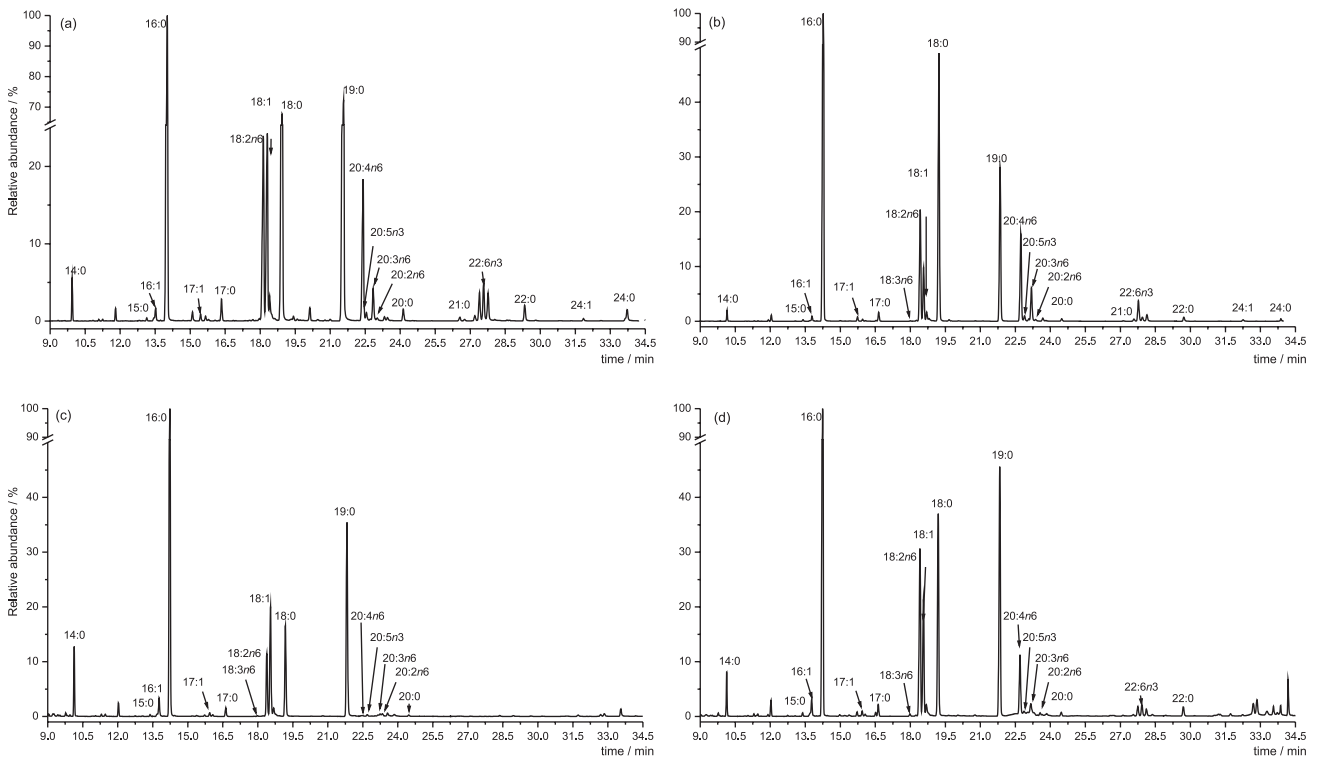


Figure S2. Representative FAME ion chromatogram showing FA present in: (a) RBCM; (b) plasma phospholipids (PL); (c) plasma triglycerides (TG) and (d) plasma cholesteryl esters (CE). Chromatographic conditions: described into CG-MS section.

The unmarked chromatographic peaks were not identified, but also do not match known fatty acid methyl esters due to different retention times and relative abundance of ions with m/z 74, 79, 81 and 87. Some fatty acid methyl esters, like 17:1 in RBCM; 21:0 in plasma phospholipids and cholesteryl esters were detected only in few samples and remained below the limit of quantification.