

Shelf-life evolution of the fatty acids fingerprint in high-quality hazelnuts (*Corylus avellana* L.) harvested in different geographical regions

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Abstract: A single paragraph of about 200 words maximum. For research articles, abstracts should give a pertinent overview of the work. We strongly encourage authors to use the following style of structured abstracts, but without headings: (1) Background: Place the question addressed in a broad context and highlight the purpose of the study; (2) Methods: briefly describe the main methods or treatments applied; (3) Results: summarize the article's main findings; (4) Conclusions: indicate the main conclusions or interpretations. The abstract should be an objective representation of the article and it must not contain results that are not presented and substantiated in the main text and should not exaggerate the main conclusions.

Keywords: keyword 1; keyword 2; keyword 3 (List three to ten pertinent keywords specific to the article yet reasonably common within the subject discipline.)

The supplementary material includes:

Supplementary Table 1 - ST1: List of FAMES standards together with their systematic names, common (trivial) names, abbreviations, reference concentration in the standard mixture, experimental and predicted relative Response Factors.

Supplementary Table 2 – ST2: Results on percentage ratio of the amount of C15:0 FAME among FFA over the EFA in all samples (30 samples x 2 extraction batches n = 60), analyzed in triplicate (60 x 3 = 180 analyses). Data adopted to normalize analytes amounts.

Supplementary Table 3 – ST3: EFAs amounts expressed as mg/g according to AOAC official method 2003.05.

Supplementary Table 4 – ST4: FFAs amounts expressed as µg/g.

Supplementary Figure 1 – SF1: Schematic diagram of the derivatization/extraction process.

Supplementary Table 1 – ST1: List of FAMES standards together with their systematic names, common (trivial) names, abbreviations, reference concentration in the standard mixture, experimental and predicted relative Response Factors.

Systematic (IUPAC) name	Common name	Shorthand (ω) name*	Shortened name	Concentration $\mu\text{g/mL}$ Reference mixture	For EFA . n-C15 ref		For FFA n-C17 ref	
					Experimental RF	RRF	Experimental RF	RRF
methylbutanoate	methylbutyrate	4:0	C4:0	419	1.497	1.493	1.284	1.526
methylhexanoate	methylcaproate	6:0	C6:0	419	0.941	1.269	0.806	1.297
methyloctanoate	methylcaprylate	8:0	C8:0	417	1.049	1.157	0.899	1.182
methyldecanoate	methyl caprate	10:0	C10:0	426	1.028	1.090	0.881	1.113
methylundecanoate	-	11:0	C11:0	215	1.033	1.065	0.885	1.088
methyldodecanoate	methyl laurate	12:0	C12:0	421	0.985	1.045	0.844	1.067
methyltridecanoate	-	13:0	C13:0	208	0.971	1.028	0.832	1.050
methyltetradecanoate	methylmyristate	10:0	C14:0	423	0.988	1.013	0.847	1.035
methylcis-9-tetradecenoate	methylmyristoleate	14:1 ω -5	C14:1 n-9	211	1.026	1.004	0.880	1.026
methylpentadecanoate	-	15:0	C15:0	209	1.000	1.000	0.857	1.022
methylcis-10-pentadecenoate	-	15:1 ω -5	C15:1 n-10	211	1.099	0.992	0.942	1.014
methylhexadecanoate	methylpalmitate	16:0	C16:0	670	1.103	0.989	0.946	1.010
methylcis-9-hexadecenoate	methylpalmitoleate	16:1 ω -7	C16:1 n-9	210	1.256	0.981	1.077	1.003
methylheptadecanoate	methylmargarate	17:0	C17:0	230	1.167	0.979	1.000	1.000
methylcis-10-heptadecanoate	-	17:1 ω -7	C17:1 n-10	210	1.075	0.972	0.922	0.993
methyloctadecanoate	methylstearate	18:0	C18:0	420	1.159	0.970	0.993	0.991
methyltrans-9-octadecenoate	methyl trans-9-elaidate	a	C18:1 n-9	212	1.233	0.964	1.057	0.984
methylcis-9-octadecenoate	methyl oleate	18:1 ω -9	C18:1n-9	422	1.248	0.964	1.070	0.984
methyl trans-9-trans-12-octadecadienoate	-	a	C18:2 n-9,12t	208	1.184	0.957	1.015	0.978
methylcis-9,cis-12-octadecadienoate	methyl linoleate	18:2 ω -6	C18:2 n-9,12	210	1.213	0.957	1.040	0.978
methylcis-6,-9,-12-octadecatrienoate	methyl γ -linolenate	18:3 ω -6	C18:3 n-6,9,12	210	1.132	0.950	0.970	0.971
methylcis-9,-12,-15-octadecatrienoate	methyl linolenate	18:3 ω 3-	C18:3 n-9,12,15	209	1.145	0.950	0.981	0.971
methyleicosanoate	methylarachidate	20:0	C20:0	420	1.262	0.955	1.082	0.976
methyl cis-11-eicosenoate	methylgondoate	20:1 ω -9	C20:1 n-11	210	1.287	0.949	1.104	0.970
methyl-cis -11,-14, eicosadienoate	methyleicosadienoate	20:2 ω -6	C20:2 n-11,14	209	1.350	0.943	1.157	0.964
methylheneicosanoate	-	21:0	C21:0	210	1.442	0.949	1.237	0.969
methylcis-8,-11,-14-eicosatrienoate	methyldihomo- γ -linolenate	20:3 ω -6	C20:3 n-8,11,14	205	1.263	0.937	1.083	0.958
methylcis-5,-8,-11,-14-eicosatetraenoate	methylarachidonate	20:4 ω -6	C20:4 n-5,8,11,14	205	1.280	0.932	1.097	0.952

Systematic (IUPAC) name	Common name	Shorthand (ω) name*	Shortened name	Concentration $\mu\text{g/mL}$ Reference mixture	For EFA		For FFA	
					Experimental RF	RRF	Experimental RF	RRF
methyl <i>cis</i> -11,14,17-eicosatrienoate	-	20:3 ω -3	C20:3 n-11,14,17	199	1.210	0.937	1.037	0.958
methyl docosanoate	methylbehenate	22:0	C22:0	422	1.374	0.943	1.178	0.963
methyl <i>cis</i> -5,-8,-11,-14,-17-eicosapentaenoate	eicosapentaenoate	20:5 ω -3	C20:5 n-5,8,11,14,17	205	1.290	0.926	1.106	0.946
methyl <i>cis</i> -13-docosenoate	methylerucate	22:1 ω -9	C22:1 n-13	210	1.389	0.938	1.191	0.958
methyltricosanoate	-	23:0	C23:0	213	0.703	0.938	1.097	0.958
methyltetracosanoate	methylignocerate	24:0	C24:0	420	1.436	0.933	1.231	0.953
methyl <i>cis</i> -15-tetracosenoate	methylnervonate	24:1 ω -9	C24:1 n-15	211	1.454	0.928	1.246	0.948
methyl <i>cis</i> -4, -7,-10,-13, -16,-19- docosahexaenoate	methyl DHA	22:6 ω -3	C22:6 n-4,7,10,13,16,19	203	1.403	0.911	1.202	0.930

*Additional methyl group for derivatization as methyl esters to be implied

Supplementary Table 2 – ST2: Results on percentage ratio of the amount of C15:0 FAME among FFA over the EFA in all samples (30 samples x 2 extraction batches n = 60), analyzed in triplicate (60 x 3 = 180 analyses). Data adopted to normalize analytes amounts.

Sample acronym	Recovery ratio %
An_Ge_E1_T0	2.24
An_Ge_E1_T12_18C	2.24
An_Ge_E1_T12_5V	2.66
An_Ge_E1_T6_18C	2.28
An_Ge_E1_T6_5V	3.27
An_Ge_E2_T0	2.84
An_Ge_E2_T12_18C	3.06
An_Ge_E2_T12_5V	4.87
An_Ge_E2_T6_18C	4.44
An_Ge_E2_T6_5V	2.81
T_Ge_E1_T0	3.60
T_Ge_E1_T12_18C	2.88
T_Ge_E1_T12_5V	2.53
T_Ge_E1_T6_18C	2.89
T_Ge_E1_T6_5V	0.87
T_Ge_E2_T0	3.22
T_Ge_E2_T12_18C	2.66
T_Ge_E2_T12_5V	2.64
T_Ge_E2_T6_18C	4.00
T_Ge_E2_T6_5V	3.52
T_It_E1_T0	2.24
T_It_E1_T12_18C	1.80
T_It_E1_T12_5V	3.85
T_It_E1_T6_18C	3.62
T_It_E1_T6_5V	3.32
T_It_E2_T0	4.21
T_It_E2_T12_18C	3.81
T_It_E2_T12_5V	2.46
T_It_E2_T6_18C	2.58
T_It_E2_T6_5V	3.95
Average (%)	3.05
Standard Deviation	0.85

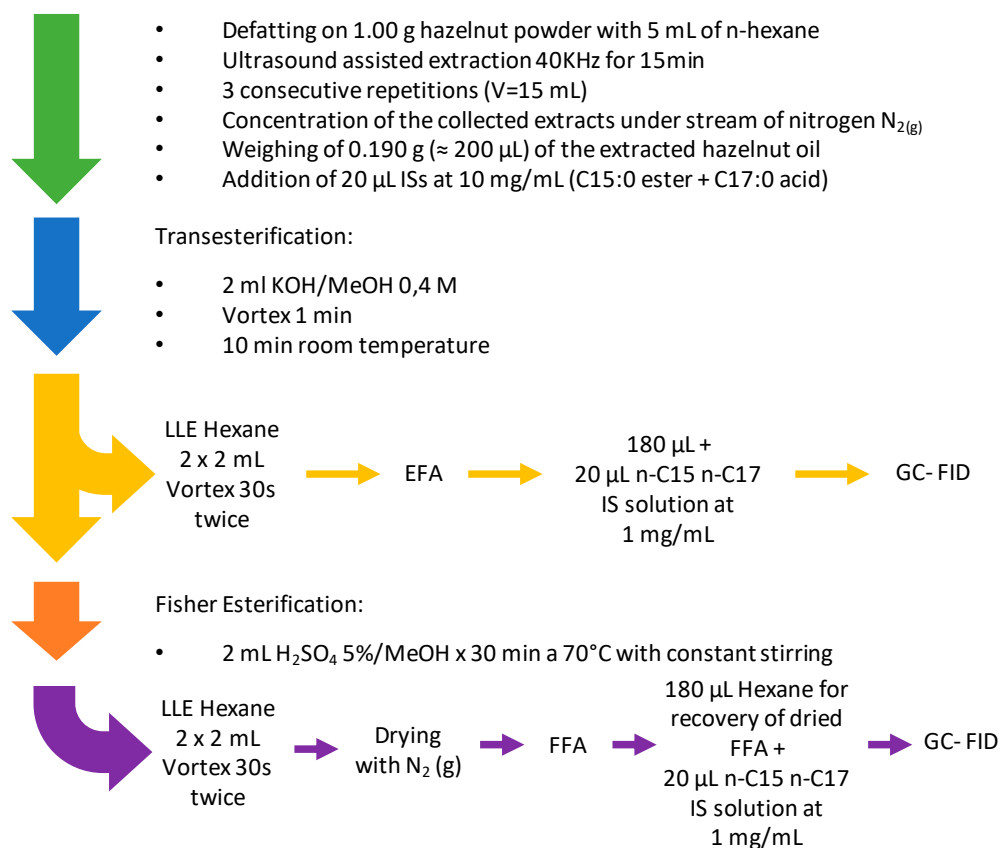
Supplementary Table 3 – ST3: EFAs amounts expressed as mg/g according to AOAC official method 2003.05.

Sample Acronym	C14:0	C16:0	C16:1	C17:1	C18:0	C18:1 n-9	C18:2 n-9,12	C18:3 n-9,12,15	C20:0	C20:1 n-15	C22:0	C22:1	C23:0	C24:0														
AN_GE_E1_T0	4.05E-02	3.47E-03	6.47E+00	4.92E-01	1.89E-01	1.60E-02	4.65E-02	2.44E-03	2.37E+00	1.51E-01	8.66E+01	5.18E+00	3.93E+00	3.68E-01	6.04E-02	3.53E-03	1.68E-01	9.55E-03	1.06E-01	2.51E-03	2.78E-02	1.82E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E-02	4.61E-04
AN_GE_E1_T12_18C	3.04E-02	2.61E-03	6.79E+00	5.16E-01	2.37E-01	2.00E-02	6.26E-02	3.28E-03	2.35E+00	1.50E-01	8.59E+01	5.14E+00	4.29E+00	4.02E-01	1.13E-02	6.58E-04	6.76E-02	3.85E-03	1.67E-01	3.94E-03	2.90E-02	1.89E-03	6.44E-02	3.84E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
AN_GE_E1_T12_5V	3.67E-02	3.14E-03	6.94E+00	5.27E-01	2.38E-01	2.01E-02	5.63E-02	2.95E-03	2.33E+00	1.49E-01	8.52E+01	5.10E+00	4.73E+00	4.43E-01	6.35E-02	3.71E-03	1.56E-01	8.91E-03	1.33E-01	3.15E-03	4.92E-02	3.22E-03	2.69E-02	1.60E-03	1.63E-02	5.56E-03	8.48E-03	3.89E-04
AN_GE_E1_T6_18C	2.13E-02	1.82E-03	6.44E+00	4.89E-01	1.08E-01	9.13E-03	3.09E-02	1.62E-03	1.35E+00	8.60E-02	8.94E+01	5.35E+00	2.35E+00	2.20E-01	3.40E-02	1.99E-03	8.46E-02	4.82E-03	7.32E-02	1.73E-03	1.83E-02	1.20E-03	4.41E-02	2.63E-03	1.15E-02	5.21E-03	1.14E-02	5.22E-04
AN_GE_E1_T6_5V	3.43E-02	2.94E-03	6.52E+00	4.96E-01	2.08E-01	1.76E-02	5.67E-02	2.97E-03	2.36E+00	1.50E-01	8.60E+01	5.15E+00	4.48E+00	4.20E-01	1.50E-02	8.77E-04	7.13E-02	4.06E-03	1.57E-01	3.71E-03	5.93E-02	3.87E-03	3.99E-02	2.38E-03	0.00E+00	0.00E+00	1.29E-02	5.91E-04
AN_GE_E2_T0	3.86E-02	3.31E-03	6.68E+00	5.08E-01	2.26E-01	1.91E-02	5.35E-02	2.80E-03	2.37E+00	1.51E-01	8.64E+01	5.17E+00	3.88E+00	3.63E-01	1.07E-02	6.27E-04	1.62E-01	9.23E-03	1.29E-01	3.06E-03	3.03E-02	1.98E-03	2.92E-02	1.74E-03	0.00E+00	0.00E+00	9.92E-03	4.55E-04
AN_GE_E2_T12_18C	3.81E-02	3.27E-03	7.14E+00	5.42E-01	2.34E-01	1.98E-02	7.03E-02	3.68E-03	2.34E+00	1.49E-01	8.54E+01	5.12E+00	4.20E+00	3.93E-01	6.40E-02	3.74E-03	1.90E-01	1.08E-02	1.81E-01	4.29E-03	3.28E-02	2.14E-03	4.42E-02	2.64E-03	1.01E-02	2.92E-03	9.67E-03	4.44E-04
AN_GE_E2_T12_5V	3.85E-02	3.30E-03	6.93E+00	5.26E-01	2.32E-01	1.97E-02	5.42E-02	2.84E-03	2.34E+00	1.49E-01	8.53E+01	5.11E+00	4.64E+00	4.35E-01	7.01E-02	4.09E-03	1.50E-01	8.52E-03	1.30E-01	3.07E-03	3.03E-02	1.98E-03	5.40E-02	3.22E-03	4.88E-03	1.55E-03	1.48E-02	6.77E-04
AN_GE_E2_T6_18C	4.12E-02	3.53E-03	6.90E+00	5.24E-01	2.51E-01	2.12E-02	5.37E-02	2.81E-03	2.32E+00	1.48E-01	8.47E+01	5.07E+00	5.34E+00	5.00E-01	7.93E-02	4.63E-03	1.63E-01	9.28E-03	1.32E-01	3.12E-03	3.03E-02	1.98E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.47E-02	6.76E-04
AN_GE_E2_T6_5V	3.12E-02	2.68E-03	6.18E+00	4.70E-01	1.79E-01	1.52E-02	5.60E-02	2.93E-03	2.37E+00	1.51E-01	8.65E+01	5.18E+00	4.32E+00	4.04E-01	7.83E-02	4.57E-03	1.53E-01	8.71E-03	1.12E-01	2.65E-03	2.04E-02	1.33E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.36E-02	6.24E-04
T_GE_E1_T0	2.76E-02	2.36E-03	7.63E+00	5.80E-01	2.84E-01	2.40E-02	5.34E-02	2.80E-03	2.35E+00	1.50E-01	8.58E+01	5.13E+00	3.53E+00	3.31E-01	1.08E-02	6.29E-04	6.10E-02	3.48E-03	1.84E-01	4.36E-03	2.99E-02	1.96E-03	5.87E-02	3.50E-03	0.00E+00	0.00E+00	1.47E-02	6.75E-04
T_GE_E1_T12_18C	1.68E-02	1.44E-03	6.13E+00	4.66E-01	1.40E-01	1.18E-02	3.88E-02	2.03E-03	1.37E+00	8.73E-02	8.90E+01	5.33E+00	3.01E+00	2.82E-01	5.10E-02	2.98E-03	8.11E-02	4.62E-03	6.99E-02	1.65E-03	2.08E-02	1.36E-03	4.77E-02	2.85E-03	1.25E-02	9.96E-03	3.86E-03	1.77E-04
T_GE_E1_T12_5V	4.45E-02	3.81E-03	7.12E+00	5.41E-01	2.78E-01	2.35E-02	5.48E-02	2.87E-03	2.36E+00	1.51E-01	8.62E+01	5.16E+00	3.48E+00	3.26E-01	5.57E-02	3.25E-03	1.70E-01	9.70E-03	1.31E-01	3.10E-03	5.03E-02	3.29E-03	3.24E-02	1.93E-03	5.51E-03	1.03E-03	3.39E-03	3.85E-04
T_GE_E1_T6_18C	3.80E-02	3.26E-03	7.26E+00	5.52E-01	2.84E-01	2.40E-02	5.41E-02	2.83E-03	2.37E+00	1.51E-01	8.65E+01	5.18E+00	3.04E+00	2.85E-01	5.70E-02	3.33E-03	1.93E-01	1.10E-02	1.27E-01	3.02E-03	5.12E-02	3.35E-03	2.82E-02	1.68E-03	0.00E+00	0.00E+00	1.36E-02	6.26E-04
T_GE_E1_T6_5V	4.52E-02	3.87E-03	6.97E+00	5.30E-01	2.63E-01	2.23E-02	6.58E-02	3.44E-03	2.38E+00	1.52E-01	8.70E+01	5.21E+00	2.94E+00	2.75E-01	1.13E-02	6.60E-04	6.39E-02	3.64E-03	1.99E-01	4.70E-03	6.29E-03	4.11E-04	4.67E-02	2.78E-03	1.24E-02	1.20E-01	7.77E-03	3.56E-04
T_GE_E2_T0	3.60E-02	3.08E-03	7.65E+00	5.81E-01	3.01E-01	2.55E-02	5.29E-02	2.77E-03	2.36E+00	1.50E-01	8.63E+01	5.16E+00	2.88E+00	2.70E-01	2.92E-02	1.71E-03	1.82E-01	1.04E-02	1.86E-01	4.39E-03	3.00E-02	1.96E-03	0.00E+00	0.00E+00	1.18E-02	5.13E-03	8.46E-03	3.88E-04
T_GE_E2_T12_18C	3.76E-02	3.22E-03	6.57E+00	5.00E-01	2.66E-01	2.25E-02	5.84E-02	3.06E-03	2.37E+00	1.51E-01	8.65E+01	5.18E+00	3.79E+00	3.55E-01	4.27E-02	2.49E-03	1.61E-01	9.16E-03	1.31E-01	3.11E-03	2.68E-02	1.75E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
T_GE_E2_T12_5V	3.06E-02	2.62E-03	1.08E+01	8.17E-01	2.51E-01	2.12E-02	4.75E-02	2.49E-03	2.27E+00	1.44E-01	8.28E+01	4.95E+00	3.47E+00	3.25E-01	3.59E-02	2.09E-03	1.46E-01	8.32E-03	1.13E-01	2.67E-03	3.73E-02	2.44E-03	5.67E-02	3.38E-03	0.00E+00	0.00E+00	2.82E-02	1.29E-03
T_GE_E2_T6_18C	4.02E-02	3.44E-03	7.19E+00	5.47E-01	2.72E-01	2.30E-02	5.00E-02	2.62E-03	2.39E+00	1.52E-01	8.71E+01	5.21E+00	2.52E+00	2.36E-01	4.13E-02	2.41E-03	1.90E-01	1.08E-02	1.26E-01	2.99E-03	3.98E-02	2.60E-03	5.38E-02	3.21E-03	1.49E-02	3.09E-03	1.50E-02	6.89E-04
T_GE_E2_T6_5V	3.89E-02	3.34E-03	7.21E+00	5.48E-01	3.15E-01	2.67E-02	5.69E-02	2.98E-03	2.36E+00	1.50E-01	8.61E+01	5.15E+00	3.39E+00	3.17E-01	4.93E-02	2.88E-03	1.92E-01	1.10E-02	1.25E-01	2.95E-03	5.96E-02	3.90E-03	9.25E-02	5.52E-03	0.00E+00	0.00E+00	1.32E-02	6.05E-04
T_IT_E1_T0	1.77E-02	1.51E-03	6.70E+00	5.09E-01	1.52E-01	1.29E-02	4.44E-02	2.33E-03	1.54E+00	9.84E-02	8.79E+01	5.26E+00	3.33E+00	3.12E-01	3.63E-02	2.12E-03	7.77E-02	4.43E-03	8.42E-02	1.99E-03	2.69E-02	1.76E-03	3.35E-02	2.00E-03	8.06E-03	1.64E-02	7.20E-03	3.30E-04
T_IT_E1_T12_18C	3.94E-02	3.37E-03	9.41E+00	7.15E-01	2.99E-01	2.53E-02	5.89E-02	3.08E-03	2.29E+00	1.46E-01	8.38E+01	5.02E+00	3.74E+00	3.50E-01	1.14E-02	6.64E-04	6.07E-02	3.46E-03	1.70E-01	4.03E-03	7.49E-03	4.89E-04	7.88E-02	4.70E-03	0.00E+00	0.00E+00	1.77E-02	8.14E-04
T_IT_E1_T12_5V	2.48E-02	2.13E-03	5.59E+00	4.25E-01	2.25E-01	1.91E-02	6.19E-02	3.24E-03	2.36E+00	1.50E-01	8.61E+01	5.15E+00	5.16E+00	4.84E-01	8.44E-02	4.92E-03	1.46E-01	8.32E-03	1.74E-01	4.11E-03	2.71E-02	1.77E-03	3.20E-02	1.91E-03	1.12E-02	6.47E-03	8.28E-03	3.80E-04
T_IT_E1_T6_18C	1.38E-02	1.19E-03	8.13E+00	6.18E-01	1.01E-01	8.52E-03	3.15E-02	1.65E-03	1.09E+00	6.97E-02	8.80E+01	5.27E+00	2.44E+00	2.29E-01	3.28E-02	1.92E-03	4.79E-02	2.73E-03	5.08E-02	1.20E-03	8.88E-03	5.80E-04	8.59E-03	5.12E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
T_IT_E1_T6_5V	2.40E-02	2.05E-03	5.98E+00	4.54E-01	2.65E-01	2.25E-02	7.10E-02	3.72E-03	2.34E+00	1.49E-01	8.55E+01	5.12E+00	5.52E+00	5.17E-01	1.31E-02	7.65E-04	9.75E-02	5.56E-03	1.30E-01	3.08E-03	2.97E-02	1.94E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.25E-02	5.72E-04
T_IT_E2_T0	2.34E-02	2.01E-03	6.22E+00	4.73E-01	2.52E-01	2.13E-02	6.29E-02	3.29E-03	2.38E+00	1.51E-01	8.67E+01	5.19E+00	4.13E+00	3.86E-01	1.49E-02	8.72E-04	7.51E-02	4.28E-03	1.44E-01	3.40E-03	2.34E-02	1.53E-03	1.54E-03	9.21E-05	2.06E-02	6.77E-03	0.00E+00	0.00E+00
T_IT_E2_T12_18C	3.19E-02	2.73E-03	6.31E+00	4.79E-01	2.31E-01	1.96E-02	6.75E-02	3.53E-03	2.36E+00	1.51E-01	8.64E+01	5.17E+00	4.25E+00	3.98E-01	1.59E-02	9.25E-04	1.37E-01	7.81E-03	1.48E-01	3.50E-03	4.09E-02	2.68E-03	3.86E-02	2.30E-03	8.04E-03	4.35E-03	1.16E-02	5.34E-04
T_IT_E2_T12_5V	2.77E-02	2.37E-03	5.79E+00	4.40E-01	2.24E-01	1.90E-02	5.66E-02	2.96E-03	2.34E+00	1.49E-01	8.55E+01	5.12E+00	5.57E+00	5.22E-01	6.68E-02	3.90E-03	1.33E-01	7.57E-03	1.22E-01	2.89E-03	4.07E-02	2.66E-03	5.90E-02	3.52E-03	1.73E-02	2.83E-03	1.61E-02	7.39E-04
T_IT_E2_T6_18C	3.04E-02	2.60E-03	6.21E+00	4.72E-01	2.29E-01	1.94E-02	5.94E-02	3.11E-03	2.35E+00	1.50E-01	8.58E+01	5.14E+00	4.76E+00	4.46E-01	7.91E-02	4.62E-03	1.63E-01	9.27E-03	1.66E-01	3.93E-03	3.39E-02	2.21E-03	3.86E-02	2.31E-03	0.00E+00	0.00E+00	5.22E-02	2.40E-03
T_IT_E2_T6_5V	2.40E-02	2.06E-03	5.75E+00	4.37E-01	2.27E-01	1.92E-02	6.01E-02	3.15E-03	2.39E+00	1.52E-01	8.70E+01	5.21E+00	4.11E+00	3.85E-01	6.88E-02	4.01E-03	1.42E-01	8.11E-03	1.48E-01	3.51E-03	3.77E-02	2.46E-03	4.97E-02	2.96E-03	0.00E+00	0.00E+00	2.09E-02	9.57E-04

Supplementary Table 4 – ST4: FFAs amounts expressed as µg/g.

Sample Acronym	C14:0		C16:0		C16:1		C17:1		C18:0		C18:1 n-9		C18:2 n-9,12		C18:3 n-9,12,15		C20:0		C22:0		C22:1		C23:0		C24:0	
AN_GE_E1_T0	6.16	± 0.53	641	± 71.22	30.80	± 1.61	7.98	± 0.51	184	± 11.02	9550	± 894.42	552	± 32.22	9.88	± 0.56	11.60	± 0.27	9.50	± 0.62	3.41	± 0.20	3.50	± 0.00	0.77	± 0.04
AN_GE_E1_T6_18C	3.83	± 0.33	451	± 38.19	17.20	± 0.90	4.68	± 0.30	105	± 6.29	11430	± 789.53	367	± 21.42	7.76	± 0.44	6.39	± 0.15	5.84	± 0.38	2.91	± 0.17	3.54	± 0.01	0.77	± 0.04
AN_GE_E1_T6_5V	6.54	± 0.56	1160	± 98.23	46.80	± 2.45	11.30	± 0.72	269	± 16.10	13900	± 1301.83	748	± 43.66	11.00	± 0.63	19.20	± 0.45	19.70	± 1.29	3.61	± 0.22	0.00	± 0.00	1.78	± 0.08
AN_GE_E1_T12_18C	6.70	± 0.57	1070	± 90.61	40.30	± 2.11	11.60	± 0.74	224	± 13.41	11600	± 1086.42	533	± 31.11	1.48	± 0.08	10.10	± 0.24	15.80	± 1.03	8.86	± 0.53	2.63	± 0.00	1.09	± 0.05
AN_GE_E1_T12_5V	5.62	± 0.48	758	± 64.19	31.90	± 1.67	9.20	± 0.59	170	± 10.18	11830	± 826.99	611	± 35.66	10.20	± 0.58	9.26	± 0.22	10.30	± 0.67	1.25	± 0.07	2.27	± 0.01	4.57	± 0.21
AN_GE_E2_T0	7.32	± 0.63	894	± 75.70	38.00	± 1.99	11.50	± 0.73	213	± 12.75	11000	± 1030.23	518	± 30.23	1.30	± 0.07	0.00	± 0.00	14.30	± 0.93	5.25	± 0.31	0.00	± 0.00	0.24	± 0.01
AN_GE_E2_T6_18C	6.37	± 0.55	952	± 80.62	37.80	± 1.98	11.50	± 0.73	215	± 12.87	11400	± 1048.96	509	± 29.71	4.49	± 0.26	14.30	± 0.34	18.80	± 1.23	15.00	± 0.90	7.41	± 0.00	4.79	± 0.22
AN_GE_E2_T6_5V	7.10	± 0.61	916	± 77.57	31.70	± 1.66	14.90	± 0.95	219	± 13.11	11400	± 1067.69	757	± 44.18	17.50	± 1.00	12.90	± 0.31	11.20	± 0.73	0.78	± 0.05	2.26	± 0.00	2.86	± 0.13
AN_GE_E2_T12_18C	14.80	± 1.27	2280	± 193.07	86.70	± 4.54	18.10	± 1.15	540	± 32.33	15000	± 1098.12	813	± 47.45	6.75	± 0.38	41.70	± 0.99	19.60	± 1.28	85.80	± 5.12	7.49	± 0.00	2.24	± 0.10
AN_GE_E2_T12_5V	7.78	± 0.67	1230	± 104.16	47.80	± 2.50	8.61	± 0.55	275	± 16.46	14200	± 1329.93	527	± 30.76	2.44	± 0.14	7.93	± 0.19	20.00	± 1.31	7.20	± 0.43	4.47	± 0.00	2.18	± 0.10
T_GE_E1_T0	6.60	± 0.57	901	± 76.30	45.00	± 2.36	11.60	± 0.74	193	± 11.55	10000	± 936.57	477	± 27.84	10.20	± 0.58	13.70	± 0.32	8.40	± 0.55	2.09	± 0.12	1.00	± 0.00	1.26	± 0.06
T_GE_E1_T6_18C	8.56	± 0.73	1180	± 99.92	55.10	± 2.89	12.50	± 0.80	262	± 15.68	13600	± 1273.73	573	± 33.44	10.80	± 0.62	20.10	± 0.48	16.70	± 1.09	6.75	± 0.40	2.97	± 0.00	2.73	± 0.13
T_GE_E1_T6_5V	7.95	± 0.68	1070	± 90.61	45.20	± 2.37	12.00	± 0.76	223	± 13.35	11600	± 1086.42	448	± 26.15	1.46	± 0.08	12.20	± 0.29	16.90	± 1.10	3.29	± 0.20	0.00	± 0.12	2.86	± 0.13
T_GE_E1_T12_18C	8.73	± 0.75	1220	± 103.31	57.90	± 3.03	10.00	± 0.64	249	± 14.91	12900	± 1208.17	691	± 40.33	4.35	± 0.25	17.30	± 0.41	16.60	± 1.09	2.93	± 0.17	0.72	± 0.01	2.80	± 0.13
T_GE_E1_T12_5V	7.09	± 0.61	1090	± 92.30	53.50	± 2.80	13.30	± 0.85	255	± 15.27	13200	± 1236.27	583	± 34.03	7.35	± 0.42	17.20	± 0.41	17.00	± 1.11	8.30	± 0.50	3.78	± 0.00	3.95	± 0.18
T_GE_E2_T0	7.23	± 0.62	971	± 82.22	49.60	± 2.60	8.85	± 0.56	211	± 12.63	11000	± 1030.23	422	± 24.63	8.67	± 0.49	14.50	± 0.34	12.10	± 0.79	2.60	± 0.16	0.00	± 0.01	2.29	± 0.11
T_GE_E2_T6_18C	9.75	± 0.84	1260	± 106.70	56.20	± 2.94	12.10	± 0.56	282	± 16.88	14600	± 1367.39	555	± 32.39	11.30	± 0.64	24.10	± 0.57	18.30	± 1.20	5.95	± 0.36	5.55	± 0.00	2.83	± 0.13
T_GE_E2_T6_5V	5.74	± 0.49	701	± 59.36	36.60	± 1.92	7.71	± 0.49	145	± 8.68	12490	± 1169.77	376	± 21.95	6.66	± 0.38	10.30	± 0.24	9.52	± 0.62	3.14	± 0.19	0.00	± 0.00	1.32	± 0.06
T_GE_E2_T12_18C	6.76	± 0.58	936	± 79.26	50.40	± 2.64	7.51	± 0.48	229	± 13.71	11900	± 1114.52	563	± 32.86	1.50	± 0.09	10.10	± 0.24	15.00	± 0.98	2.29	± 0.14	0.00	± 0.00	1.10	± 0.05
T_GE_E2_T12_5V	4.49	± 0.38	576	± 48.78	26.90	± 1.41	4.41	± 0.28	131	± 7.84	16770	± 1570.63	367	± 21.42	5.46	± 0.31	7.69	± 0.18	8.10	± 0.53	2.85	± 0.17	2.50	± 0.00	1.00	± 0.05
T_IT_E1_T0	2.50	± 0.21	334	± 28.28	18.60	± 0.97	4.30	± 0.27	100	± 5.99	9200	± 955.30	389	± 22.70	5.08	± 0.29	4.29	± 0.10	9.39	± 0.61	2.63	± 0.16	2.47	± 0.02	5.01	± 0.23
T_IT_E1_T6_18C	5.97	± 0.51	856	± 72.49	33.60	± 1.76	7.81	± 0.50	224	± 13.41	11600	± 1086.42	508	± 29.65	8.15	± 0.46	9.42	± 0.22	8.53	± 0.56	5.43	± 0.32	4.26	± 0.00	4.07	± 0.19
T_IT_E1_T6_5V	4.53	± 0.39	868	± 73.50	38.40	± 2.01	13.40	± 0.85	238	± 14.25	12300	± 1151.98	607	± 35.43	1.82	± 0.10	8.67	± 0.21	17.00	± 1.11	10.90	± 0.65	3.47	± 0.01	3.59	± 0.16
T_IT_E1_T12_18C	2.45	± 0.21	332	± 28.11	16.80	± 0.88	4.21	± 0.27	104	± 6.23	15410	± 1443.25	406	± 23.70	6.34	± 0.36	5.15	± 0.12	6.44	± 0.42	2.58	± 0.15	0.00	± 0.00	6.86	± 0.31
T_IT_E1_T12_5V	4.87	± 0.42	966	± 81.80	52.10	± 2.73	10.40	± 0.66	273	± 16.34	14100	± 1320.56	1150	± 67.12	1.59	± 0.09	0.00	± 0.00	13.00	± 0.85	1.88	± 0.11	0.00	± 0.00	2.05	± 0.09
T_IT_E2_T0	6.62	± 0.57	532	± 78.92	49.20	± 2.58	16.70	± 1.06	266	± 15.92	9800	± 1292.47	567	± 33.09	8.39	± 0.48	16.00	± 0.38	1.44	± 0.09	3.00	± 0.18	0.01	± 0.01	3.41	± 0.16
T_IT_E2_T6_18C	5.32	± 0.46	759	± 64.27	35.70	± 1.87	12.30	± 0.78	204	± 12.21	10600	± 992.76	811	± 47.33	12.30	± 0.70	11.70	± 0.28	13.50	± 0.88	8.66	± 0.52	3.95	± 0.00	3.35	± 0.15
T_IT_E2_T6_5V	4.65	± 0.40	738	± 62.49	37.10	± 1.94	10.90	± 0.69	191	± 11.43	9880	± 925.33	772	± 45.06	8.80	± 0.50	10.40	± 0.25	13.30	± 0.87	3.28	± 0.20	1.79	± 0.00	0.92	± 0.04
T_IT_E2_T12_18C	7.39	± 0.63	916	± 77.57	28.90	± 1.51	12.90	± 0.82	249	± 14.91	12900	± 1208.17	573	± 33.44	1.82	± 0.10	10.40	± 0.25	13.60	± 0.89	6.11	± 0.36	5.03	± 0.00	3.53	± 0.16
T_IT_E2_T12_5V	5.84	± 0.50	902	± 76.38	44.00	± 2.30	12.50	± 0.80	236	± 14.13	12200	± 1142.61	1030	± 60.12	13.90	± 0.79	11.30	± 0.27	17.30	± 1.13	2.27	± 0.14	3.36	± 0.00	2.71	± 0.12

Supplementary Figure 1 – SF1: Schematic diagram of the derivatization/extraction process.



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