Lipid profiling: Proving the geographical origin of strawberries (*Fragaria* × *ananassa*) using a non-targeted LC-IM-MS approach

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Table S1: Sample information of all measured strawberry samples with their geographical origin (partly with the region), harvest year and variety.

Number	State	Region	Year	Variety
1	Greece	Westgriechenland	2022	Not specified
2	Spain	Valencia	2022	Fortuna
3	Spain	Huelva	2022	Not specified
4	Spain	Huelva	2022	Not specified
5	Spain	Valencia	2022	Not specified
6	Netherlands	Not specified	2022	Not specified
7	Netherlands	Holland	2022	Not specified
8	Spain	Huelva	2022	Not specified
9	Spain	Not specified	2022	Not specified
10	Spain	Huelva	2022	Not specified
11	Netherlands	Not specified	2022	Not specified
12	Germany	Hessen	2022	Not specified
13	Germany	Hessen	2022	Clery
14	Germany	Hessen	2022	Lady Emma
15	Germany	Hessen	2022	Clery
16	Germany	Hessen	2022	Not specified
17	Germany	Baden-Württemberg	2022	Aprica
18	Germany	Baden-Württemberg	2022	Aprica
19	Germany	Baden-Württemberg	2022	Clery
20	Germany	Baden-Württemberg	2022	Clery
21	Germany	Baden-Württemberg	2022	Asia
22	Germany	Baden-Württemberg	2022	Clery
23	Germany	Baden-Württemberg	2022	Sonsation
24	Germany	Baden-Württemberg	2022	Sibilla
25	Germany	Baden-Württemberg	2022	Clery
26	Germany	Baden-Württemberg	2022	Asia
27	Germany	Baden-Württemberg	2022	Not specified
28	Germany	Baden-Württemberg	2022	Not specified
29	Germany	Bayern	2022	Alegro
30	Germany	Bayern	2022	Not specified
31	Germany	Bayern	2022	Not specified
32	Germany	Bayern	2022	Asia
33	Germany	Bayern	2022	Clery
34	Germany	Bayern	2022	Limalexia
35	Germany	Bayern	2022	Sonata
36	Germany	Thüringen	2022	Rumba
37	Germany	Thüringen	2022	Kimberly
38	Germany	Thüringen	2022	Not specified
39	Germany	Niedersachsen	2022	Malwina
40	Germany	Niedersachsen	2022	Faith
41	Germany	Niedersachsen	2022	Faith
42	Germany	Niedersachsen	2022	Sonata
43	Germany	Niedersachsen	2022	Faith
44	Netherlands	Not specified	2022	Not specified
45	Greece	Nea Manolada	2022	Not specified
46	Greece	Not specified	2022	Not specified
47	Greece	Nea Manolada	2023	Not specified
48	Spain	Huelva	2023	Not specified
49	Spain	Huelva	2023	Not specified
50	Greece	Westgriechenland	2023	Not specified
51	Spain	Huelva	2023	Not specified
52	Spain	Huelva	2023	Not specified
53	Spain	Huelva	2023	Felicity

Number	State	Region	Year	Variety
54	Egypt	Not specified	2023	Not specified
55	Spain	Huelva	2023	Not specified
56	Spain	Andalusien	2023	Not specified
57	Egypt	Not specified	2023	Not specified
58	Spain	Huelva	2023	Not specified
59	Spain	Huelva	2023	Not specified
60	Egypt	Not specified	2023	Fortuna
61	Spain	Huelva	2023	Victory
62	Egypt	Not specified	2023	Fortuna
63	Greece	Westgriechenland	2023	Not specified
64	Spain	Andalusien	2023	Rociera
65	Spain	Andalusien	2023	Calinda
66	Spain	Andalusien	2023	Not specified
67	Spain	Andalusien	2023	Not specified
68	Greece	ZentralmakkedoNiedersachsenen	2023	Victory
69	Greece	Westgriechenland	2023	Calderon
70	Greece	Westgriechenland	2023	Not specified
71	Greece	Westgriechenland	2023	Not specified
72	Greece	Westgriechenland	2023	Not specified
73	Greece	Westgriechenland	2023	Not specified
74	Spain	Andalusien	2023	Not specified
75	Spain	Andalusien	2023	Calinda
76	Greece	Westgriechenland	2023	Not specified
77	Spain	Andalusien	2023	Not specified
78	Greece	Westgriechenland	2023	Not specified
79	Netherlands	Gelderland	2023	Malling Centenary
80	Netherlands	Limburg	2023	Elsanta
81	Netherlands	Gelderland	2023	Malling Centenary
82	Netherlands	Not specified	2023	Sonata
83	Spain	Andalusien	2023	Not specified
84	Greece	Westgriechenland	2023	Not specified
85	Egypt	Not specified	2023	Not specified
86	Egypt	Not specified	2023	Not specified
87	Egypt	Not specified	2023	Not specified
88	Egypt	Not specified	2023	Not specified
89	Egypt	Not specified	2023	Not specified
90	Netherlands	Limburg	2023	Not specified
91	Germany	Hessen	2023	Not specified
92	Germany	Hessen	2023	Faith
93	Germany	Hessen	2023	Not specified
94	Germany	Baden-Württemberg	2023	Verdi
95	Germany	Baden-Württemberg	2023	Thear
96	Germany	Baden-Württemberg	2023	Sonata
97	Germany	Baden-Württemberg	2023	Sonsation
98	Germany	Bayern	2023	Lambada
99	Germany	Bayern	2023	Salsa
100	Germany	Niedersachsen	2023	Not specified
101	Germany	Niedersachsen	2023	Not specified
102	Germany	Niedersachsen	2023	Not specified
103	Netherlands	Not specified	2023	Not specified
104	Netherlands	Limburg	2023	Not specified
105	Netherlands	Gelderland	2023	Elsanta
106	Netherlands	Limburg	2023	Opera

Number	State	Region	Year	Variety
107	Netherlands	Not specified	2023	Not specified
108	Greece	Westgriechenland	2023	Not specified
109	Egypt	Not specified	2023	Not specified
110	Egypt	Not specified	2023	Not specified
111	Egypt	Not specified	2023	Not specified
112	Egypt	Not specified	2023	Not specified
113	Egypt	Not specified	2023	Not specified
114	Egypt	Not specified	2023	Not specified
115	Egypt	Not specified	2023	Not specified
116	Egypt	Not specified	2023	Not specified
117	Polen	Not specified	2023	Not specified
118	Polen	Not specified	2023	Not specified
119	Polen	Not specified	2023	Not specified
120	Polen	Not specified	2023	Not specified
121	Polen	Not specified	2023	Not specified
122	Polen	Not specified	2023	Not specified
123	Polen	Not specified	2023	Not specified
124	Spain	Huelva	2024	Not specified
125	Spain	Huelva	2024	Not specified
126	Spain	Huelva	2024	Felicity
127	Spain	Huelva	2024	Not specified
128	Netherlands	Not specified	2024	Sonsation
129	Spain	Huelva	2024	Not specified
130	Greece	Not specified	2024	Fortuna
131	Spain	Huelva	2024	Rabida
132	Netherlands	Not specified	2024	Inspire
133	Egypt	Not specified	2024	Not specified
134	Greece	Westgriechenland	2024	Not specified
135	Spain	Huelva	2024	Not specified
136	Greece	Westgriechenland	2024	Not specified
137	Egypt	Not specified	2023	Not specified
138	Egypt	Not specified	2023	Not specified
139	Egypt	Not specified	2023	Not specified
140	Egypt	Not specified	2023	Not specified
141	Egypt	Not specified	2023	Not specified
142	Egypt	Not specified	2023	Not specified
143	Egypt	Not specified	2023	Not specified
144	Egypt	Not specified	2023	Not specified
145	Egypt	Not specified	2023	Not specified
146	Egypt	Not specified	2023	Not specified
147	Egypt	Not specified	2023	Not specified
148	Polen	Not specified	2023	Not specified
149	Polen	Not specified	2023	Not specified
150	Polen	Not specified	2023	Not specified
151	Polen	Not specified	2023	Not specified
152	Polen	Not specified	2023	Not specified
153	Greece	Not specified	2024	Not specified
154	Greece	Not specified	2024	Not specified
155	Greece	Westgriechenland	2024	Not specified
156	Netherlands	Limburg	2024	Elsanta
157	Netherlands	Gelderland	2024	Lady Emma
158	Netherlands	Not specified	2024	Not specified
159	Spain	Not specified	2024	Not specified
160	Germany	Baden-Württemberg	2024	Not specified
161	Polen	Not specified	2024	Not specified

Number	State	Region	Year	Variety
162	Polen	Not specified	2024	Not specified
163	Polen	Not specified	2024	Not specified
164	Polen	Not specified	2024	Not specified
165	Polen	Not specified	2024	Not specified
166	Polen	Not specified	2024	Hademar
167	Polen	Not specified	2024	Not specified
168	Polen	Not specified	2024	Hademar
169	Polen	Not specified	2024	Not specified
170	Polen	Not specified	2024	Not specified
171	Polen	Not specified	2024	Hademar
172	Polen	Not specified	2024	Flair
173	Polen	Not specified	2024	Not specified
174	Germany	Hessen	2024	Wima Zanta
175	Germany	Hessen	2024	Sonsation
176	Germany	Hessen	2024	Clery
177	Germany	Baden-Württemberg	2024	Asia
178	Netherlands	Not specified	2024	Not specified
179	Netherlands	Not specified	2024	Not specified
180	Netherlands	Not specified	2024	Not specified
181	Netherlands	Not specified	2024	Not specified
182	Netherlands	Not specified	2024	Not specified
183	Netherlands	Not specified	2024	Not specified
184	Netherlands	Not specified	2024	Not specified
185	Netherlands	Not specified	2024	Not specified
186	Netherlands	Not specified	2024	Not specified
187	Netherlands	Not specified	2024	Not specified
188	Netherlands	Not specified	2024	Not specified
189	Netherlands	Not specified	2024	Not specified
190	Netherlands	Not specified	2024	Not specified
191	Netherlands	Not specified	2024	Not specified
192	Germany	Niedersachsen	2024	Not specified
193	Polen	Not specified	2024	Not specified
194	Polen	Not specified	2024	Not specified
195	Polen	Not specified	2024	Hademar

Table S2: Chromatography gradient for the LC-MS measurements of the strawberry extracts. Both solvents had an addition of 0.1 mMol/L ammonium formate.

Time [min]	Water [%]	Isopropanol/Acetonitril (2:1, v/v) [%]
0	35	65
2	35	65
4	15	85
22	0	100
23	0	100
25	35	65
30	35	65

Table S3: Confusion matrix of the LDA classification results for distinguishing the strawberry samples according to their variety.

		Predicted						
	Class	Asia [%]	Clery [%]	Faith [%]	Fortuna [%]	Hademar [%]	Sonsation [%]	Specificity [%]
True	Asia [%]	26.0	48.8	1.8	0.0	1.3	22.3	99.0
	Clery [%]	1.8	97.1	1.1	0.0	0.0	0.0	52.7
	Faith [%]	0.0	72.8	25.3	0.0	0.0	2.0	97.9
	Fortuna [%]	0.0	0.0	0.0	100.0	0.0	0.0	100.0
	Hademar [%]	0.5	72.3	1.8	0.0	0.5	25.0	92.3
	Sonsation [%]	2.3	43.0	6.8	0.0	45.3	2.8	91.8
	Sensitivity [%]	26.0	97.1	25.3	100.0	0.5	2.8	50.3

Table S4: Confusion matrix of the LDA classification results for distinguishing the strawberry samples according to their harvest year.

		Predicted			
	Class	2022 [%]	2023 [%]	2024 [%]	Specificity [%]
True	2022 [%]	50.4	28.0	21.5	76.4
	2023 [%]	25.8	51.6	22.6	51.6
	2024 [%]	20.0	35.5	44.5	64.5
	Sensitivity [%]	60.4	72.4	61.1	56.4

Table S5: Summary of identification parameters for the marker compounds selected by ANOVA (*p*-value < 0.01). In the following table, the letters "TG" stands for triglycerides, "DG" for diacylglycerides, "PC" for phosphatidylcholines, "FDR" for false discovery rate, "RT" for retention time, "DT" for Drift time and "CCS" for cross collision section.

Tentative Metabolite	*p*-value	FDR	Sum formula	Ion	*m/z* (analytical)	*m/z* (calculated)	Δ *m/z* [Da]	RT [min]	DT [ms]	CCS-value (analytical) [Å]	CCS-value (LipidCCS database) [Å]	Main fragments [*m/z*]
TG 60:5	4.49e-05	4.56e-05	$C_{63}H_{112}O_6$	+H	965.8538	965.8532	0.0006	18.6	45.58	337.2	336.8-341.7	263.25 265.25 597.45
TG 18:1_22:0_18:3	3.69e-05	3.69e-05	$C_{61}H_{112}O_6$	+H	956.8672	956.8641	0.0031	17.2	45.38	333.8	333.6	261.25 599.50
TG 18:0_18:3_22:0	2.67e-07	5.35e-06	$C_{61}H_{112}O_6$	$+NH_4$	958.8817	958.8797	0.002	17.9	45.34	335.4	334.8	265.25 601.54
TG 18:0_18:3_22:0	2.31e-08	6.21e-07	$C_{61}H_{112}O_6$	+Na	963.8346	963.8351	0.0004	17.9	45.61	333.5	333.1	261.25 601.51
TG 18:0_18:2_22:0	9.05e-07	1.42e-05	$C_{61}H_{114}O_6$	$+NH_4$	960.8949	960.8954	0.0005	18.6	45.82	335.0	334.3	263.25 603.54
TG 18:0_18:1_22:0	8.48e-06	1.06e-04	$C_{61}H_{116}O_6$	$+NH_4$	962.9092	962.9110	0.0018	19.9	43.33	333.5	334.1	265.25 605.55 663.63
TG 56:6	6.94e-08	1.65e-06	$C_{59}H_{102}O_6$	+H	907.7756	907.7749	0.0007	13.3	43.63	325.0	325.7	265.25 603.50
TG 18:1_20:0_18:3	8.86e-05	8.23e-04	$C_{59}H_{106}O_6$	$+NH_4$	928.8326	928.8328	0.0002	16.4	44.68	328.7	328.8	261.25 599.50
TG 20:0_18:2_18:1	4.59e-14	4.37e-12	$C_{59}H_{108}O_6$	$+NH_4$	930.8484	930.8484	0.0001	18.01	44.87	330.1	330.3	601.52 263.23
TG 18:1_20:0_18:1	3.79e-20	1.15e-17	$C_{59}H_{110}O_6$	+Na	937.8192	937.8195	0.0003	17.9	44.85	331.9	331.4	603.54 265.25
TG 18:1_20:0_18:1	1.23e-14	1.34e-12	$C_{59}H_{110}O_6$	$+NH_4$	932.8689	932.8641	0.0048	18.3	45.08	329.7	328.7	263.25 575.51
TG 18:1_18:1_18:1	1.95e-07	4.17e-06	$C_{57}H_{104}O_6$	$+NH_4$	902.8169	902.8171	0.0003	16.3	44.12	325.6	325.7	265.25 603.54
TG 18:2_18:0_18:0	4.02e-08	1.02e-06	$C_{57}H_{106}O_6$	$+NH_4$	904.8326	904.8326	0.0002	17.1	44.29	326.9	326.5	263.25 603.53
TG 52:7	1.04e-04	9.56e-04	$C_{55}H_{92}O_6$	$+NH_4$	866.7232	866.7186	0.0046	11.9	42.04	310.4	310.1	577.55
TG	3.89e-	6.94e-	$C_{55}H_{94}O_6$	$+NH_4$	870.7580	870.7545	0.0035	16.7	42.66	315.9	315.3	261.25

Tentative Metabolite	*p*-value	FDR	Sum formula	Ion	*m/z* (analytical)	*m/z* (calculated)	Δ *m/z* [Da]	RT [min]	DT [ms]	CCS-value (analytical) [Å]	CCS-value (LipidCCS database) [Å]	Main fragments [*m/z*]
52:5	07	06										597.45
TG 16:0_18:1_18:1	2.30e-07	4.77e-06	$C_{55}H_{102}O_6$	$+NH_4$	876.8015	876.8015	0.0001	16.3	43.49	320.1	320.7	265.25 603.54
TG 18:3_18:1_15:0	5.57e-04	5.56e-04	$C_{54}H_{96}O_6$	+Na	863.7047	863.7099	0.0052	12.6	40.62	312.8	313.2	261.25 265.25 595.47
PC 40:7	1.13e-04	1.02e-02	$C_{48}H_{82}NO_8P$	$+H\text{-}H_2O$	814.5713	814.5751	0.0064	5.3	39.43	296.2	296.2	184.07
PC 38:6	5.01e-16	6.90e-14	$C4_6H_{80}NO_8P$	+H	806.5659	806.5694	0.0035	7.9	39.69	290.2	290.7	184.07
PC 38:5	2.37e-28	3.60e-25	$C_{46}H_{82}NO_8P$	+H	808.5853	808.5851	0.0002	8.9	39.86	293.5	293.3	184.07
PC 36:6	1.24e-08	3.57e-07	$C_{44}H_{76}NO_8P$	+Na	800.5191	800.5201	0.001	6.3	38.36	284.3	285.1	184.07
PC 36:6	3.66e-07	6.79e-06	$C_{44}H_{76}NO_8P$	+H	778.5414	778.5381	0.0033	7.3	38.59	284.1	284.8	184.07
PC 36:5	2.12e-11	1.15e-09	$C_{44}H_{78}NO_8P$	+H	780.5562	780.5538	0.0024	7.9	39.00	289.2	289.1	184.07
PC 36:4	1.99e-05	2.28e-03	$C_{44}H_{80}NO_8P$	+Na	804.5482	804.5514	0.0032	7.2	39.30	290.3	287.0-290.2	184.07
PC 36:4	1.00e-07	2.27e-06	$C_{44}H_{80}NO_8P$	+H	782.5670	782.5694	0.0024	7.2	38.81	287.8	286.8-288.9	184.07
PC 36:3	1.77e-17	3.37e-15	$C_{44}H_{82}NO_8P$	+H	784.5823	784.5851	0.0028	7.8	39.22	290.8	290.6	184.07
PC 36:2	1.20e-25	9.12e-23	$C_{44}H_{84}NO_8P$	+H	786.5995	786.6007	0.0012	8.9	39.44	292.5	292.4	184.08
PC 36:1	5.58e-05	5.52e-04	$C_{44}H_{86}NO_8P$	+Na	810.5954	810.5983	0.0029	10.1	39.95	296.1	295.9-297.8	184.07
PC 36:1	2.09e-11	1.15e-09	$C_{44}H_{86}NO_8P$	+H	788.6136	788.6164	0.0028	10.1	39.61	293.7	293.9	184.07
PC 35:2	2.81e-08	7.25e-07	$C_{43}H_{82}NO_8P$	+H	772.5834	772.5851	0.0017	8.5	38.97	289.0	289.8	184.07
PC 34:3	2.27e-	2.52e-	$C_{42}H_{78}NO$	+H	756.5528	756.5538	0.001	7.3	38.07	282.4	283.5	184.07

Tentative Metabolite	*p*-value	FDR	Sum formula	Ion	*m/z* (analytical)	*m/z* (calculated)	Δ *m/z* [Da]	RT [min]	DT [ms]	CCS-value (analytical) [Å]	CCS-value (LipidCCS database) [Å]	Main fragments [*m/z*]
	05	04	$_8$P									
PC 34:2	3.92e-07	6.94e-06	$C_{42}H_{80}NO_8P$	+H	758.5681	758.5694	0.0013	7.8	38.54	285.9	286.6-288.4	184.07
PC 34:1	1.03e-10	4.50e-09	$C_{42}H_{82}NO_8P$	+H	760.5836	760.5851	0.0015	8.8	38.81	289.9	289.5	184.07
PC 33:4	2.69e-13	2.15e-11	$C_{41}H_{74}NO_8P$	+H	740.5253	740.5225	0.0028	7.1	36.93	281.0	281.3	184.07
PC 33:3	1.77e-11	1.03e-09	$C_{41}H_{76}NO_8P$	+Na	764.5179	764.5201	0.0022	7.1	37.98	281.7	282.9	184.07
PC 33:3	2.97e-06	4.13e-05	$C_{41}H_{76}NO_8P$	+H	742.5360	742.5381	0.0021	6.9	37.31	281.8	282.7	184.07
PC 33:2	1.64e-05	1.92e-07	$C_{41}H_{78}NO_8P$	+Na	766.5326	766.5357	0.0031	8.0	38.49	285.5	285.3	184.07
PC 32:1	8.51e-05	7.95e-04	$C_{40}H_{78}NO_8P$	+H	732.5511	732.5538	0.0027	8.5	37.91	284.4	284.7-286.5	184.07
LPC 16:0	1.04e-14	1.22e-12	$C_{24}H_{50}NO_7P$	+H	496.3477	496.3398	0.0079	3.1	30.74	229.8	226.9-232.3	184.07
LPC 18:2	8.36e-11	3.88e-09	$C_{26}H_{50}NO_7P$	+H	520.3379	520.3398	0.0019	2.9	27.96	233.6	233.6	184.07
DG 18:1_18:4	4.11e-16	6.25e-14	$C_{39}H_{66}O_5$	+H	615.5062	615.4983	0.0079	8.4	34.67	258.0	257.4-260.3	599.50 261.22
DG 18:1_18:2	8.07e-07	1.32e-05	$C_{39}H_{70}O_5$	+H-H_2O	601.5174	601.5196	0.0022	15.5	34.74	261.0	261.6	265.25
DG 16:0_18:3	1.19e-05	1.44e-04	$C_{37}H_{66}O_5$	+Na	613.4796	613.4802	0.0006	6.8	33.77	256.3	256.1	261.22 595.47
DG (16:0_18:1)	3.09e-06	4.32e-05	$C_{37}H_{70}O_5$	+H-H_2O	577.5173	577.5196	0.0023	4.6	34.62	262.22	262.5	265.25
DG (15:0_18:2)	3.59e-07	6.75e-06	$C_{37}H_{68}O_5$	+H-H_2O	575.5016	575.5040	0.0024	7.3	34.26	257.4	257.9	263.24

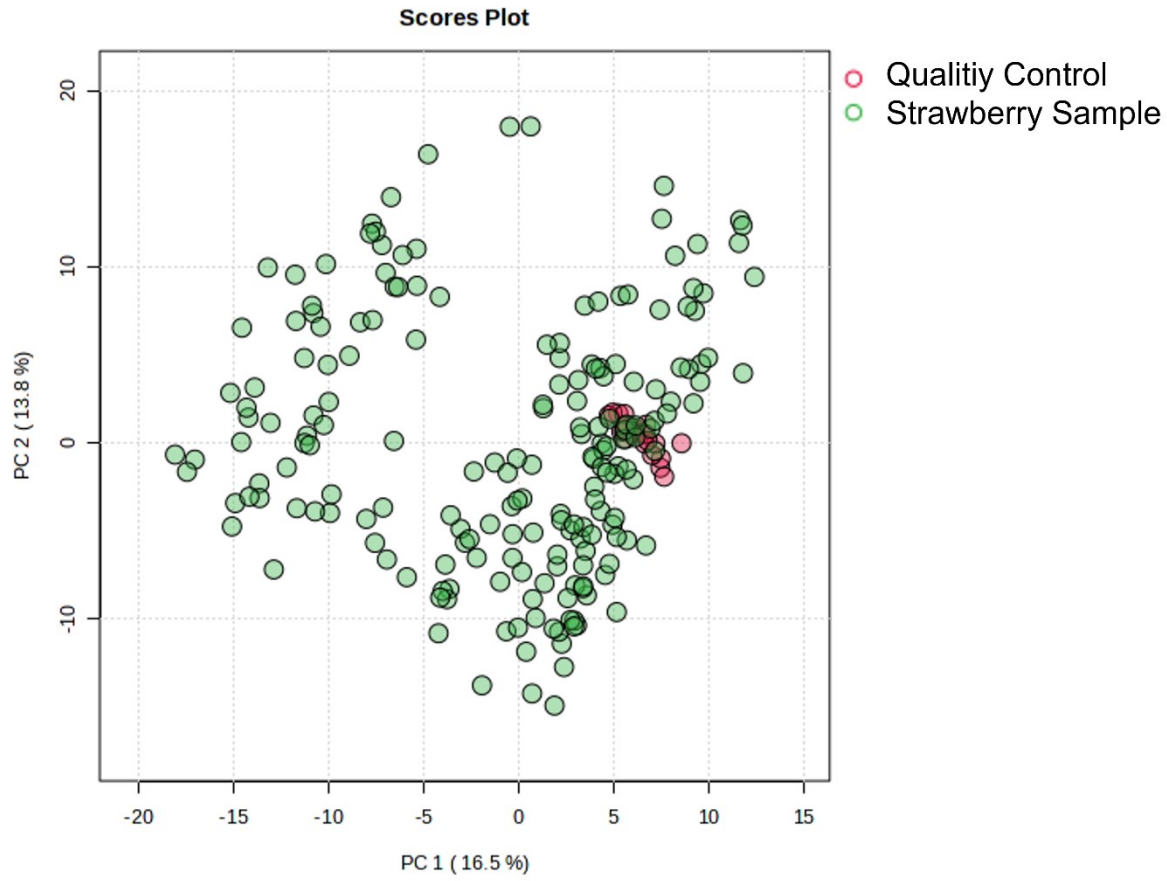

Figure S1: Result of the PCA score plot of PC1 and PC2 of the 195 strawberry samples (green dots) and the measurements of the 22 QC samples (red dots). The data were sum normalized and scaled.

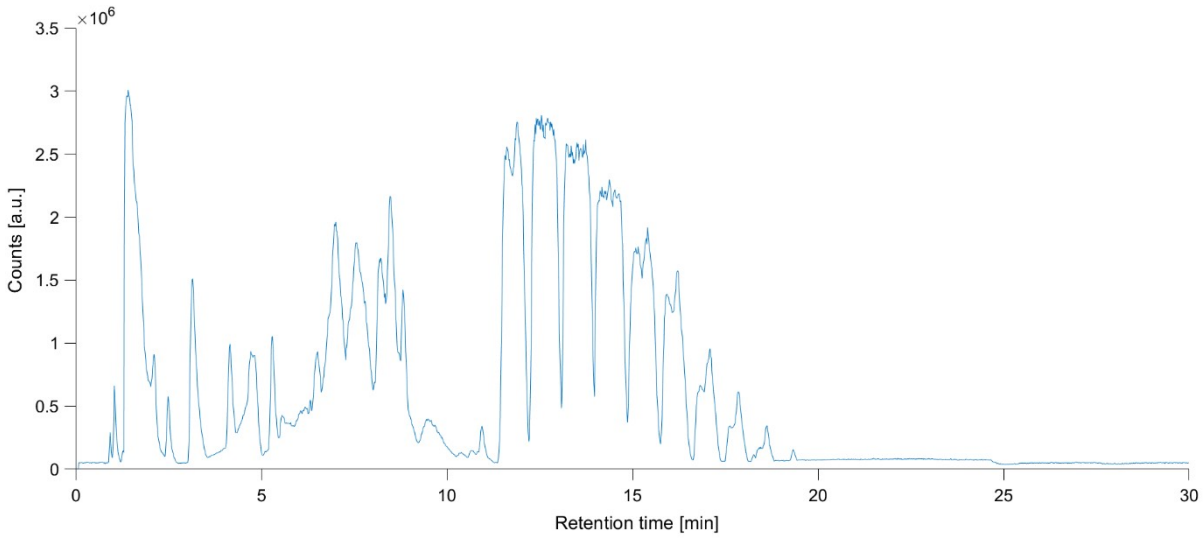

Figure S2: Example of a total ion chromatogram of a measurement from a strawberry QC sample.

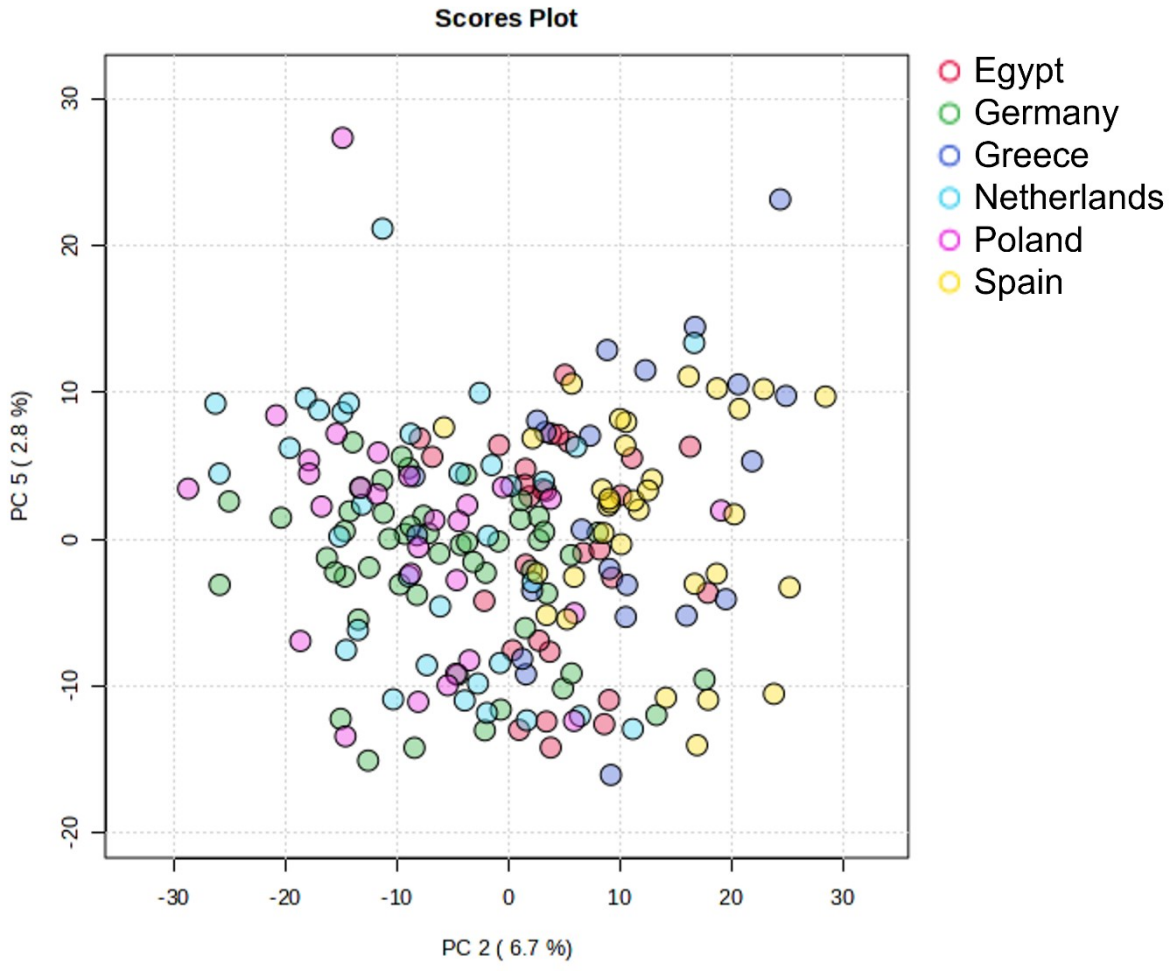

Figure S3: Score plots of PC2 and PC5, to distinguish the geographical origin from German, Polish, Dutch, Spanish, Greek and Egyptian strawberries.

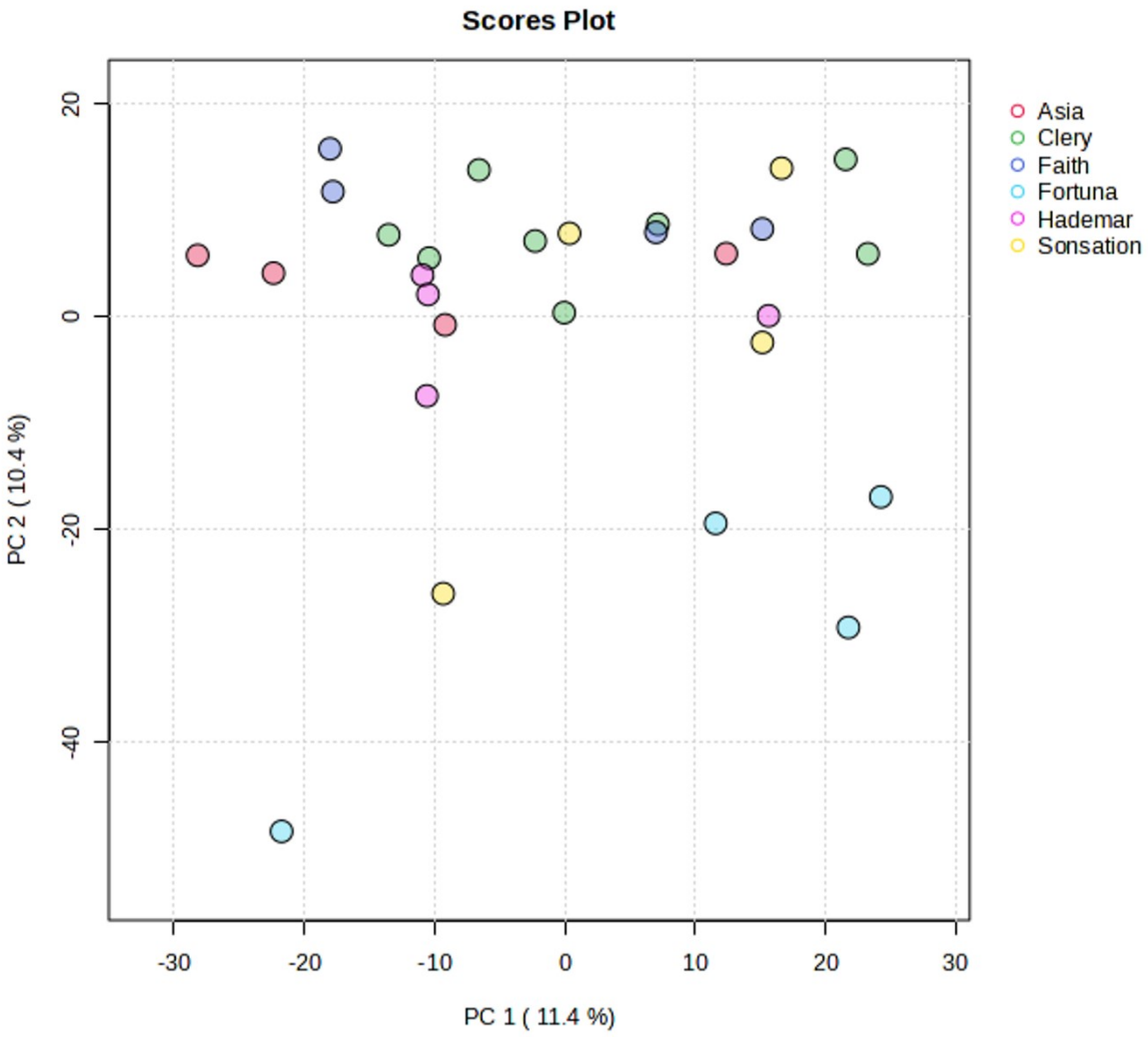

Figure S4: Score plots of PC1 and PC2, to analyze the effect of the variety on the geographical origin of the strawberries.

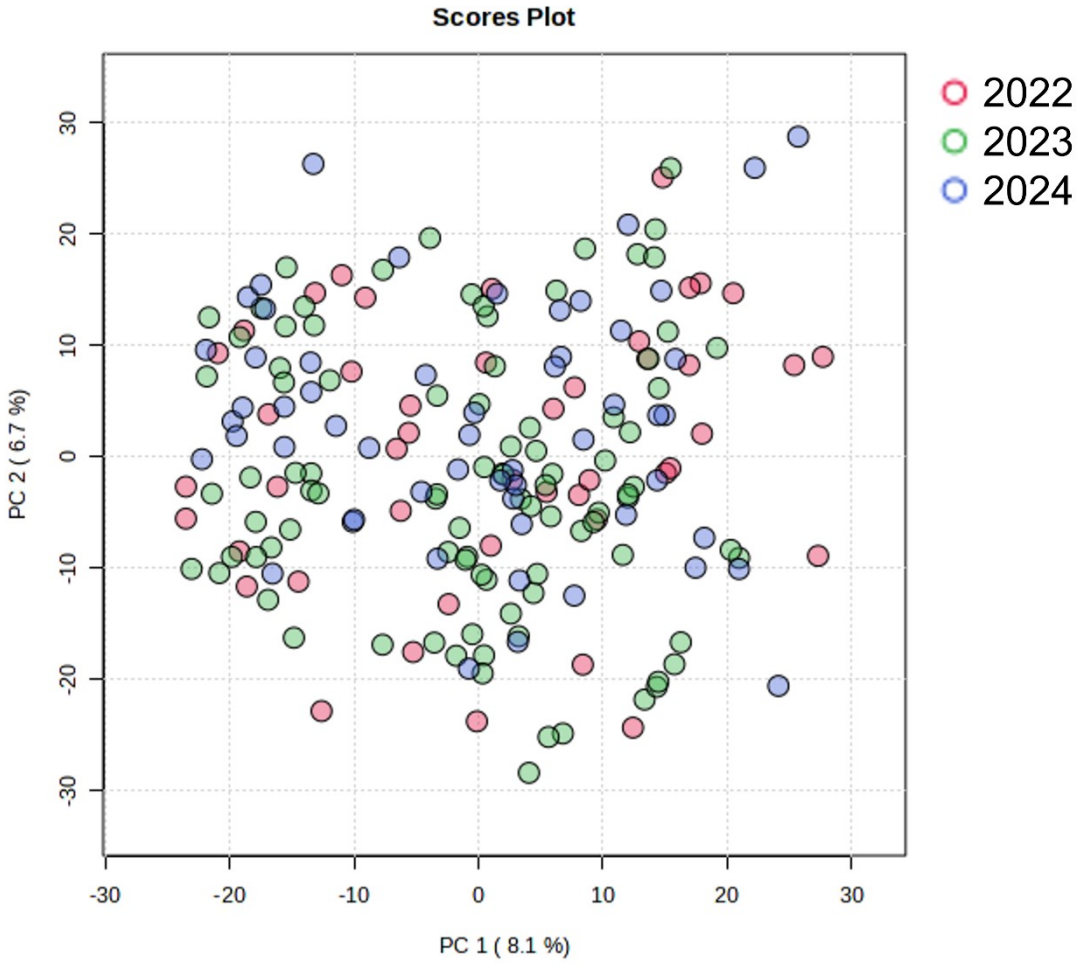

Figure S5: Score plots of PC1 and PC2, to analyze the effect of the harvest years on the geographical origin of the strawberries.

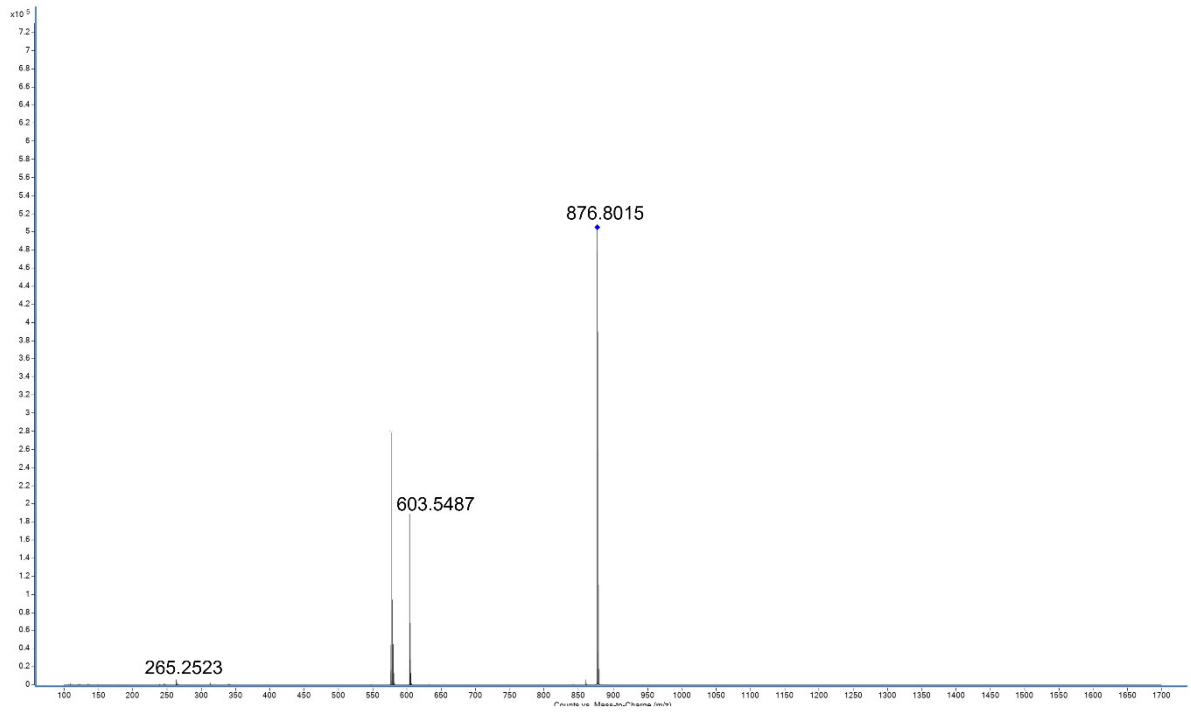

Figure S5: MS/MS spectrum of the signal *m*/*z* 876.8015 at a retention time of 16.3 min in a strawberry sample extract. The collision energy was 40 eV. The compound was identified as TG 16:0_18:1_18:1.

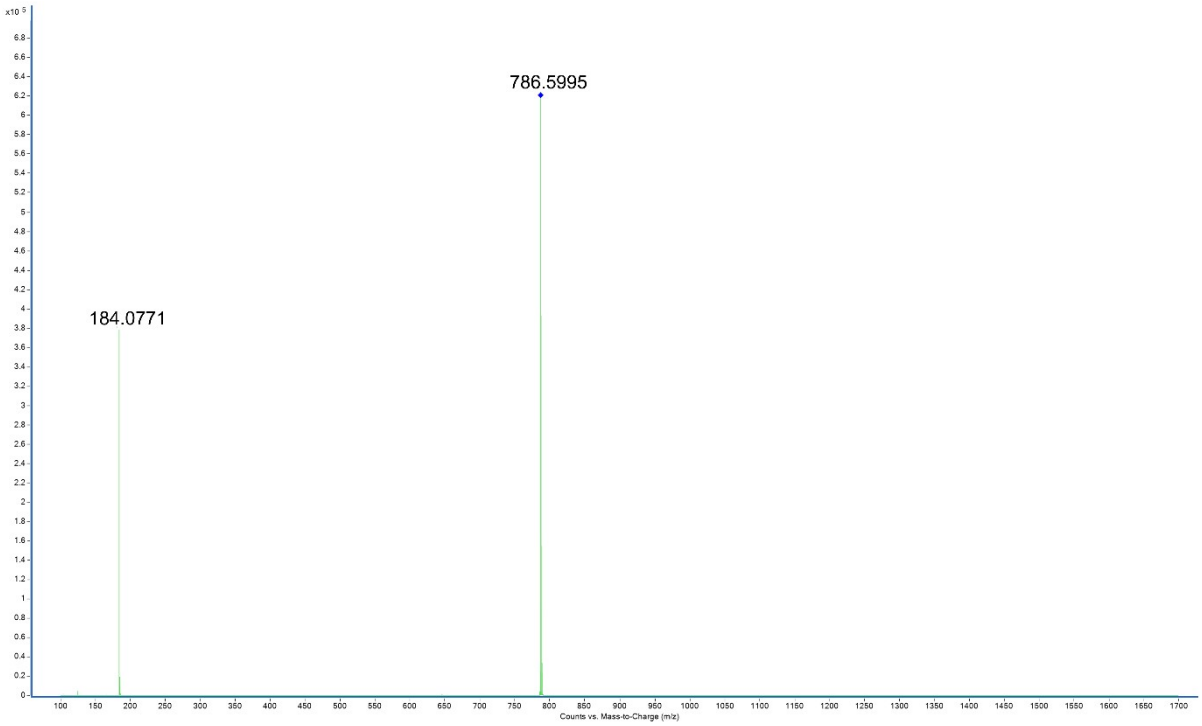

Figure S5: MS/MS spectrum of the signal *m*/*z* 786.5995 at a retention time of 8.9 min in a strawberry sample extract. The collision energy was 20 eV. The compound was identified as PC 36:2.

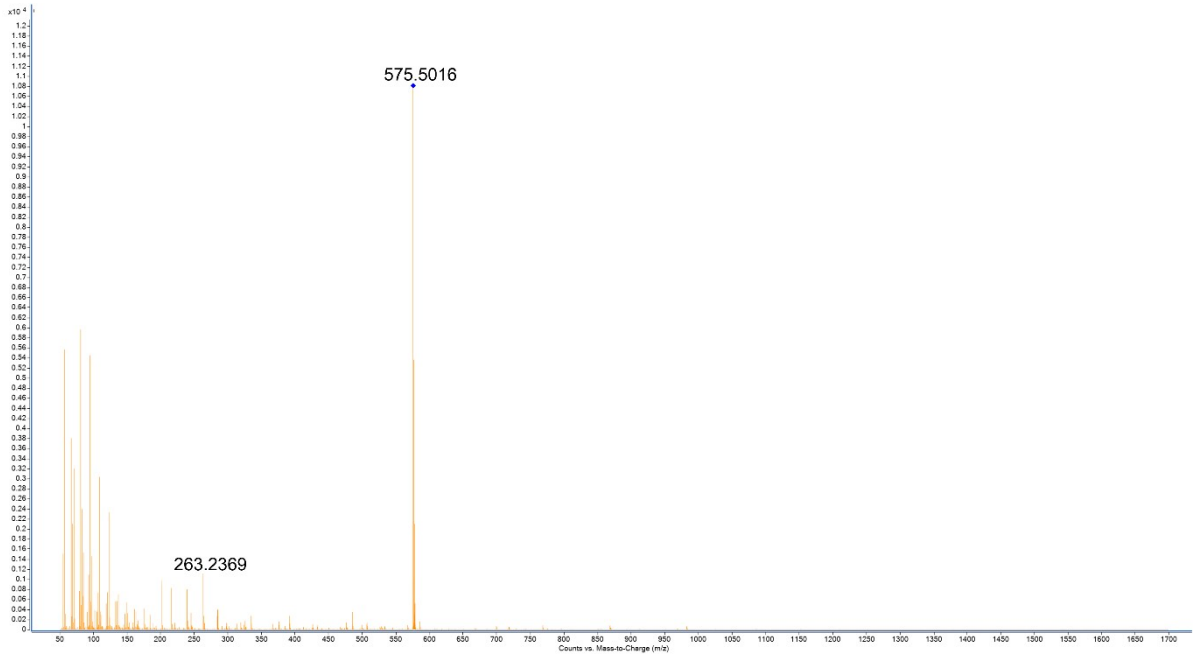

Figure S5: MS/MS spectrum of the signal *m*/*z* 575.5016 at a retention time of 7.3 min in a strawberry sample extract. The collision energy was 20 eV. The compound was identified as DG 15:0_18:2.