

Supplementary material

Table S1 Lipid molecular species in 13 different types of vegetable oils and animal fats

No.	Lipid ion	<i>m/z</i> (Calc)	<i>m/z</i> (Obs)	Ion formula	Retention time(min)
1	LPC(18:2) + H	520.3398	520.3322	C ₂₆ H ₅₁ O ₇ N ₁ P ₁	0.79
2	LPC(18:2) + H	520.3398	520.3326	C ₂₆ H ₅₁ O ₇ N ₁ P ₁	0.87
3	PC(34:3) + H	756.5538	756.5535	C ₄₂ H ₇₉ O ₈ N ₁ P ₁	12.54
4	DG(18:3/18:2) + NH ₄	632.5249	632.5242	C ₃₉ H ₇₀ O ₅ N ₁	12.63
5	PC(24:0/12:4) + H	782.5694	782.5694	C ₄₄ H ₈₁ O ₈ N ₁ P ₁	12.72
6	DG(18:1/18:3) + NH ₄	634.5405	634.5399	C ₃₉ H ₇₂ O ₅ N ₁	13.65
7	DG(18:1/18:2) + NH ₄	636.5562	636.5552	C ₃₉ H ₇₄ O ₅ N ₁	14.71
8	AcHexCmE(14:0) + NH ₄	790.6555	790.6552	C ₄₈ H ₈₈ O ₇ N ₁	15.40
9	DG(18:1/18:1) + NH ₄	638.5718	638.5713	C ₃₉ H ₇₆ O ₅ N ₁	15.73
10	AcHexSiE(14:0) + NH ₄	804.6712	804.6712	C ₄₉ H ₉₀ O ₇ N ₁	15.91
11	AcHexCmE(18:2) + NH ₄	842.6868	842.6862	C ₅₂ H ₉₂ O ₇ N ₁	15.94
12	DG(18:1/18:2) + H	619.5296	619.5273	C ₃₉ H ₇₁ O ₅	16.55
13	TG(16:0/18:1/18:3) + H	855.7436	855.7430	C ₅₅ H ₉₉ O ₆	18.52
14	TG(18:3/18:2/18:3) + NH ₄	892.7389	892.7391	C ₅₇ H ₉₈ O ₆ N ₁	19.03
15	TG(14:0/14:0/18:3) + NH ₄	790.6919	790.6919	C ₄₉ H ₉₂ O ₆ N ₁	19.31
16	TG(12:0/18:2/18:2) + NH ₄	816.7076	816.7075	C ₅₁ H ₉₄ O ₆ N ₁	19.38
17	TG(18:2/14:1/18:2) + NH ₄	842.7232	842.7232	C ₅₃ H ₉₆ O ₆ N ₁	19.44
18	TG(16:0/18:3/18:3) + NH ₄	868.7389	868.7383	C ₅₅ H ₉₈ O ₆ N ₁	19.51
19	TG(18:3/18:2/18:2) + NH ₄	894.7545	894.7550	C ₅₇ H ₁₀₀ O ₆ N ₁	19.65
20	TG(18:3/17:1/18:2) + NH ₄	882.7545	882.7544	C ₅₆ H ₁₀₀ O ₆ N ₁	19.90
21	TG(15:0/18:2/18:3) + NH ₄	856.7389	856.7387	C ₅₄ H ₉₈ O ₆ N ₁	20.07
22	TG(10:0/18:1/18:1) + NH ₄	792.7076	792.7080	C ₄₉ H ₉₄ O ₆ N ₁	20.14
23	TG(18:1/12:0/18:2) + NH ₄	818.7232	818.7236	C ₅₁ H ₉₆ O ₆ N ₁	20.22
24	TG(16:0/18:2/18:3) + NH ₄	870.7545	870.7539	C ₅₅ H ₁₀₀ O ₆ N ₁	20.28
25	TG(18:2/18:2/18:2) + NH ₄	896.7702	896.7703	C ₅₇ H ₁₀₂ O ₆ N ₁	20.33
26	TG(18:1/13:0/18:2) + NH ₄	832.7389	832.7388	C ₅₂ H ₉₈ O ₆ N ₁	20.59
27	TG(18:1/13:0/18:2) + NH ₄	832.7389	832.7389	C ₅₂ H ₉₈ O ₆ N ₁	20.67
28	TG(15:0/18:2/18:2) + NH ₄	858.7545	858.7553	C ₅₄ H ₁₀₀ O ₆ N ₁	20.69
29	TG(18:2/17:1/18:2) + NH ₄	884.7702	884.7710	C ₅₆ H ₁₀₂ O ₆ N ₁	20.74
30	TG(18:2/18:2/18:2) + NH ₄	896.7702	896.7706	C ₅₇ H ₁₀₂ O ₆ N ₁	20.77
31	TG(18:2/18:2/18:2) + H	879.7436	879.7441	C ₅₇ H ₉₉ O ₆	20.84
32	TG(16:0/18:2/18:2) + NH ₄	872.7702	872.7700	C ₅₅ H ₁₀₂ O ₆ N ₁	21.11
33	TG(15:0/16:0/18:2) + NH ₄	834.7545	834.7546	C ₅₂ H ₁₀₀ O ₆ N ₁	21.23
34	TG(18:1/18:1/18:3) + NH ₄	898.7858	898.7858	C ₅₇ H ₁₀₄ O ₆ N ₁	21.27
35	TG(15:0/18:1/18:2) + NH ₄	860.7702	860.7703	C ₅₄ H ₁₀₂ O ₆ N ₁	21.45
36	TG(18:1/17:1/18:2) + NH ₄	886.7858	886.7860	C ₅₆ H ₁₀₄ O ₆ N ₁	21.48
37	TG(20:1/18:2/18:3) + NH ₄	924.8015	924.8016	C ₅₉ H ₁₀₆ O ₆ N ₁	21.50
38	TG(16:0/14:0/18:1) + NH ₄	822.7545	822.7546	C ₅₁ H ₁₀₀ O ₆ N ₁	21.53

39	TG(19:1/18:2/18:2) + NH ₄	912.8015	912.8013	C ₅₈ H ₁₀₆ O ₆ N ₁	21.70
40	TG(16:0/16:0/18:2) + NH ₄	848.7702	848.7702	C ₅₃ H ₁₀₄ O ₆ N ₁	21.71
41	TG(16:0/18:1/18:2) + NH ₄	874.7858	874.7858	C ₅₅ H ₁₀₄ O ₆ N ₁	21.90
42	TG(15:0/16:0/18:1) + NH ₄	836.7702	836.7701	C ₅₂ H ₁₀₂ O ₆ N ₁	22.03
43	TG(18:1/18:1/18:2) + NH ₄	900.8015	900.8013	C ₅₇ H ₁₀₆ O ₆ N ₁	22.08
44	TG(20:1/18:2/18:2) + NH ₄	926.8171	926.8170	C ₅₉ H ₁₀₈ O ₆ N ₁	22.09
45	TG(15:0/18:1/18:1) + NH ₄	862.7858	862.7860	C ₅₄ H ₁₀₄ O ₆ N ₁	22.16
46	TG(18:1/17:1/18:1) + NH ₄	888.8015	888.8015	C ₅₆ H ₁₀₆ O ₆ N ₁	22.21
47	TG(16:0/16:0/18:1) + NH ₄	850.7858	850.7858	C ₅₃ H ₁₀₄ O ₆ N ₁	22.31
48	TG(19:1/18:1/18:2) + NH ₄	914.8171	914.8173	C ₅₈ H ₁₀₈ O ₆ N ₁	22.39
49	TG(16:0/18:1/18:1) + NH ₄	876.8015	876.8015	C ₅₅ H ₁₀₆ O ₆ N ₁	22.40
50	TG(18:1/18:1/18:1) + NH ₄	902.8171	902.8173	C ₅₇ H ₁₀₈ O ₆ N ₁	22.63
51	TG(22:0/18:2/18:3) + NH ₄	954.8484	954.8478	C ₆₁ H ₁₁₂ O ₆ N ₁	22.80
52	TG(17:0/18:1/18:1) + NH ₄	890.8171	890.8174	C ₅₆ H ₁₀₈ O ₆ N ₁	22.87
53	TG(16:0/16:0/16:0) + NH ₄	824.7702	824.7699	C ₅₁ H ₁₀₂ O ₆ N ₁	22.92
54	TG(18:2/18:2/21:0) + NH ₄	942.8484	942.8484	C ₆₀ H ₁₁₂ O ₆ N ₁	22.99
55	TG(19:1/18:1/18:1) + NH ₄	916.8328	916.8328	C ₅₈ H ₁₁₀ O ₆ N ₁	23.00
56	TG(18:0/16:0/18:1) + NH ₄	878.8171	878.8171	C ₅₅ H ₁₀₈ O ₆ N ₁	23.04
57	TG(18:0/18:1/18:1) + NH ₄	904.8328	904.8325	C ₅₇ H ₁₁₀ O ₆ N ₁	23.12
58	TG(18:0/16:0/16:0) + NH ₄	852.8015	852.8012	C ₅₃ H ₁₀₆ O ₆ N ₁	23.18
59	TG(18:1/18:2/22:1) + NH ₄	956.8641	956.8635	C ₆₁ H ₁₁₄ O ₆ N ₁	23.38
60	TG(24:1/18:2/18:2) + NH ₄	982.8797	982.8798	C ₆₃ H ₁₁₆ O ₆ N ₁	23.46
61	TG(19:0/18:1/18:1) + NH ₄	918.8484	918.8485	C ₅₈ H ₁₁₂ O ₆ N ₁	23.51
62	TG(16:0/18:1/19:0) + NH ₄	892.8328	892.8328	C ₅₆ H ₁₁₀ O ₆ N ₁	23.52
63	TG(18:1/18:2/21:0) + NH ₄	944.8641	944.8637	C ₆₀ H ₁₁₄ O ₆ N ₁	23.56
64	TG(18:2/18:2/23:0) + NH ₄	970.8797	970.8793	C ₆₂ H ₁₁₆ O ₆ N ₁	23.61
65	TG(20:0/16:0/18:1) + NH ₄	906.8484	906.8484	C ₅₇ H ₁₁₂ O ₆ N ₁	23.63
66	TG(20:0/16:0/16:0) + NH ₄	880.8328	880.8328	C ₅₅ H ₁₁₀ O ₆ N ₁	23.80
67	TG(20:0/18:1/18:1) + NH ₄	932.8641	932.8634	C ₅₉ H ₁₁₄ O ₆ N ₁	23.87
68	TG(18:1/18:1/22:1) + NH ₄	958.8797	958.8790	C ₆₁ H ₁₁₆ O ₆ N ₁	23.95
69	TG(18:1/18:2/24:1) + NH ₄	984.8954	984.8954	C ₆₃ H ₁₁₈ O ₆ N ₁	24.02
70	TG(16:0/18:1/21:0) + NH ₄	920.8641	920.8641	C ₅₈ H ₁₁₄ O ₆ N ₁	24.10
71	TG(18:1/18:1/21:0) + NH ₄	946.8797	946.8796	C ₆₀ H ₁₁₆ O ₆ N ₁	24.10
72	TG(18:1/18:2/23:0) + NH ₄	972.8954	972.8954	C ₆₂ H ₁₁₈ O ₆ N ₁	24.26
73	TG(25:0/18:2/18:2) + NH ₄	998.9110	998.9110	C ₆₄ H ₁₂₀ O ₆ N ₁	24.27
74	TG(26:0/18:2/18:2) + NH ₄	1012.9267	1012.9258	C ₆₅ H ₁₂₂ O ₆ N ₁	24.38
75	TG(18:1/18:1/22:0) + NH ₄	960.8954	960.8948	C ₆₁ H ₁₁₈ O ₆ N ₁	24.48
76	TG(18:1/18:2/24:0) + NH ₄	986.9110	986.9106	C ₆₃ H ₁₂₀ O ₆ N ₁	24.55
77	TG(16:0/18:1/23:0) + NH ₄	948.8954	948.8955	C ₆₀ H ₁₁₈ O ₆ N ₁	24.73
78	TG(18:1/18:1/23:0) + NH ₄	974.9110	974.9111	C ₆₂ H ₁₂₀ O ₆ N ₁	24.79
79	TG(25:0/18:1/18:2) + NH ₄	1000.9267	1000.9268	C ₆₄ H ₁₂₂ O ₆ N ₁	24.85
80	TG(26:0/18:1/18:2) + NH ₄	1014.9423	1014.9423	C ₆₅ H ₁₂₄ O ₆ N ₁	24.86
81	TG(16:0/18:1/24:0) + NH ₄	962.9110	962.9108	C ₆₁ H ₁₂₀ O ₆ N ₁	24.92
82	TG(16:0/16:0/24:0) + NH ₄	936.8954	936.8959	C ₅₉ H ₁₁₈ O ₆ N ₁	24.99

83	TG(18:1/18:1/24:0) + NH ₄	988.9267	988.9257	C ₆₃ H ₁₂₂ O ₆ N ₁	25.01
84	TG(28:1/18:1/18:2) + NH ₄	1040.9580	1040.9580	C ₆₇ H ₁₂₆ O ₆ N ₁	25.26
85	TG(25:0/16:0/18:1) + NH ₄	976.9267	976.9269	C ₆₂ H ₁₂₂ O ₆ N ₁	25.27
86	TG(25:0/18:1/18:1) + NH ₄	1002.9423	1002.9422	C ₆₄ H ₁₂₄ O ₆ N ₁	25.28
87	TG(26:0/16:0/18:1) + NH ₄	990.9423	990.9424	C ₆₃ H ₁₂₄ O ₆ N ₁	25.50
88	TG(26:0/18:1/18:1) + NH ₄	1016.9580	1016.9580	C ₆₅ H ₁₂₆ O ₆ N ₁	25.56
89	TG(28:0/18:1/18:2) + NH ₄	1042.9736	1042.9736	C ₆₇ H ₁₂₈ O ₆ N ₁	25.59
90	TG(30:1/18:1/18:2) + NH ₄	1068.9893	1068.9898	C ₆₉ H ₁₃₀ O ₆ N ₁	25.72
91	TG(28:0/16:0/18:1) + NH ₄	1018.9736	1018.9736	C ₆₅ H ₁₂₈ O ₆ N ₁	26.00
92	TG(28:0/18:1/18:1) + NH ₄	1044.9893	1044.9893	C ₆₇ H ₁₃₀ O ₆ N ₁	26.01
93	TG(30:0/18:1/18:1) + NH ₄	1073.0206	1073.0204	C ₆₉ H ₁₃₄ O ₆ N ₁	26.50

Table S2 Potential biomarkers for distinguishing between fresh olive oil and fresh sunflower oil

No.	Lipid ion	Ion formula	Retention time (min)	Notes
1	TG(16:0/16:0/16:0) + NH ₄	C ₅₁ H ₁₀₂ O ₆ N ₁	19.99	Potential biomarkers of olive oil
2	TG(18:1/17:1/18:1) + NH ₄	C ₅₆ H ₁₀₆ O ₆ N ₁	22.38	
3	TG(16:0/18:1/18:1) + NH ₄	C ₅₅ H ₁₀₆ O ₆ N ₁	22.45	
4	TG(17:0/18:1/18:1) + NH ₄	C ₅₆ H ₁₀₈ O ₆ N ₁	22.99	
5	TG(18:2/18:2/23:0) + NH ₄	C ₆₂ H ₁₁₆ O ₆ N ₁	23.66	Potential biomarkers of sunflower oil
6	TG(20:0/16:0/18:1) + NH ₄	C ₅₇ H ₁₁₂ O ₆ N ₁	23.76	
7	TG(18:1/18:2/24:0) + NH ₄	C ₆₃ H ₁₂₀ O ₆ N ₁	24.34	
8	TG(16:0/18:1/24:0) + NH ₄	C ₆₁ H ₁₂₀ O ₆ N ₁	24.96	

Table S3 Potential biomarkers for distinguishing between fresh soybean oil and fresh palm oil

No.	Lipid ion	Ion formula	Retention time (min)	Notes
1	TG(16:0/16:0/16:0) + NH ₄	C ₅₁ H ₁₀₂ O ₆ N ₁	22.92	Potential biomarkers of palm oil
2	TG(18:0/16:0/18:1) + NH ₄	C ₅₅ H ₁₀₈ O ₆ N ₁	23.27	
3	TG(20:0/16:0/16:0) + NH ₄	C ₅₅ H ₁₁₀ O ₆ N ₁	25.29	
4	TG(16:0/16:0/24:0) + NH ₄	C ₅₉ H ₁₁₈ O ₆ N ₁	26.18	
5	TG(16:0/18:1/18:1) + NH ₄	C ₅₅ H ₁₀₆ O ₆ N ₁	22.38	Potential biomarkers of soybean oil
6	TG(19:0/18:1/18:1) + NH ₄	C ₅₈ H ₁₁₂ O ₆ N ₁	23.51	
7	TG(18:1/18:2/21:0) + NH ₄	C ₆₀ H ₁₁₄ O ₆ N ₁	23.56	
8	TG(18:2/18:2/23:0) + NH ₄	C ₆₂ H ₁₁₆ O ₆ N ₁	23.61	

Table S4 Potential biomarkers for distinguishing between fresh peanut oil and fresh linseed oil

No.	Lipid ion	Ion formula	Retention time (min)	Notes
1	TG(20:0/18:1/18:1) + NH ₄	C ₅₉ H ₁₁₄ O ₆ N ₁	23.85	Potential biomarkers of peanut oil
2	TG(30:0/18:1/18:1) + NH ₄	C ₆₉ H ₁₃₄ O ₆ N ₁	26.50	
3	TG(18:1/17:1/18:1) + NH ₄	C ₅₆ H ₁₀₆ O ₆ N ₁	22.31	Potential biomarkers of linseed oil
4	TG(19:1/18:1/18:1) + NH ₄	C ₅₈ H ₁₁₀ O ₆ N ₁	23.00	
5	TG(16:0/18:1/21:0) + NH ₄	C ₅₈ H ₁₁₄ O ₆ N ₁	24.19	
6	TG(25:0/16:0/18:1) + NH ₄	C ₆₂ H ₁₂₂ O ₆ N ₁	25.24	

Table S5 Potential biomarkers for distinguishing between fresh peanut oil and fresh linseed oil

No.	Lipid ion	Ion formula	Retention time (min)	Notes
1	TG(16:0/14:0/18:1) + NH ₄	C ₅₁ H ₁₀₀ O ₆ N ₁	21.67	Potential biomarkers of castor oil
2	TG(16:0/16:0/16:0) + NH ₄	C ₅₁ H ₁₀₂ O ₆ N ₁	22.45	
3	TG(18:0/16:0/16:0) + NH ₄	C ₅₃ H ₁₀₆ O ₆ N ₁	23.18	
4	TG(20:0/16:0/16:0) + NH ₄	C ₅₅ H ₁₁₀ O ₆ N ₁	23.76	
5	TG(18:1/18:1/21:0) + NH ₄	C ₆₀ H ₁₁₆ O ₆ N ₁	24.21	Potential biomarkers of tung oil
6	TG(18:1/18:2/23:0) + NH ₄	C ₆₂ H ₁₁₈ O ₆ N ₁	24.22	
7	TG(18:1/18:1/23:0) + NH ₄	C ₆₂ H ₁₂₀ O ₆ N ₁	24.71	
8	TG(25:0/18:1/18:2) + NH ₄	C ₆₄ H ₁₂₂ O ₆ N ₁	24.77	

Table S6 Potential biomarkers for distinguishing between fresh sheep oil and fresh lard

No.	Lipid ion	Ion formula	Retention time (min)	Notes
1	TG(16:0/14:0/18:1) + NH ₄	C ₅₁ H ₁₀₀ O ₆ N ₁	21.53	Potential biomarkers of sheep oil
2	TG(15:0/16:0/18:1) + NH ₄	C ₅₂ H ₁₀₂ O ₆ N ₁	22.03	
3	TG(18:1/18:1/23:0) + NH ₄	C ₆₂ H ₁₂₀ O ₆ N ₁	24.67	
4	TG(26:0/18:1/18:1) + NH ₄	C ₆₅ H ₁₂₆ O ₆ N ₁	25.02	
5	TG(18:1/17:1/18:2) + NH ₄	C ₅₆ H ₁₀₄ O ₆ N ₁	21.48	Potential biomarkers of lard
6	TG(20:1/18:2/18:3) + NH ₄	C ₅₉ H ₁₀₆ O ₆ N ₁	21.50	
7	TG(20:1/18:2/18:2) + NH ₄	C ₅₉ H ₁₀₈ O ₆ N ₁	22.09	
8	TG(20:0/16:0/16:0) + NH ₄	C ₅₅ H ₁₁₀ O ₆ N ₁	23.80	

Table S7 Potential biomarkers for distinguishing between fresh butter and fresh duck oil

No.	Lipid ion	Ion formula	Retention time (min)	Notes
1	TG(15:0/16:0/18:1) + NH ₄	C ₅₂ H ₁₀₂ O ₆ N ₁	22.03	Potential biomarkers of butter
2	TG(15:0/18:1/18:1) + NH ₄	C ₅₄ H ₁₀₄ O ₆ N ₁	22.27	
3	TG(18:1/17:1/18:1) + NH ₄	C ₅₆ H ₁₀₆ O ₆ N ₁	22.31	
4	TG(16:0/16:0/24:0) + NH ₄	C ₅₉ H ₁₁₈ O ₆ N ₁	24.86	
5	PC(34:3) + H	C ₄₂ H ₇₉ O ₈ N ₁ P ₁	12.54	Potential biomarkers of duck oil
6	AcHexSIE(14:0) + NH ₄	C ₄₉ H ₉₀ O ₇ N ₁	15.91	
7	TG(19:0/18:1/18:1) + NH ₄	C ₅₈ H ₁₁₂ O ₆ N ₁	23.22	
8	TG(16:0/14:0/18:1) + NH ₄	C ₅₁ H ₁₀₀ O ₆ N ₁	24.47	

Table S8 Potential biomarkers for distinguishing between fresh olive oil and fresh lard

No.	Lipid ion	Ion formula	Retention time (min)	Notes
1	TG(16:0/16:0/16:0) + NH ₄	C ₅₁ H ₁₀₂ O ₆ N ₁	19.99	Potential biomarkers of olive oil
2	TG(18:1/18:1/22:0) + NH ₄	C ₆₁ H ₁₁₈ O ₆ N ₁	24.56	
3	TG(26:0/16:0/18:1) + NH ₄	C ₆₃ H ₁₂₄ O ₆ N ₁	25.52	
4	TG(26:0/18:1/18:1) + NH ₄	C ₆₅ H ₁₂₆ O ₆ N ₁	25.59	
5	TG(15:0/18:1/18:1) + NH ₄	C ₅₄ H ₁₀₄ O ₆ N ₁	22.16	Potential biomarkers of lard
6	TG(20:0/16:0/16:0) + NH ₄	C ₅₅ H ₁₁₀ O ₆ N ₁	23.80	
7	TG(16:0/16:0/24:0) + NH ₄	C ₅₉ H ₁₁₈ O ₆ N ₁	24.99	