

An untargeted lipidomic approach for qualitative determination of latent fingerprint glycerides using UPLC-IMS-QToF-MSE

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Supporting information

Glyceride standard	Glyceride structure	Average retention time (min)	Average experimental m/z ($[M+H-H_2O]^+$)	Average CCS (\AA^2) ($[M+H-H_2O]^+$)	Average experimental m/z ($[M+Na]^+$)	Average CCS (\AA^2) ($[M+Na]^+$)
Dimyristin	DG 14:0_14:0	7.18	495.4409	253.2	535.4332	248.3
Dipalmitolein	DG 16:1_16:1	7.71	547.4724	260.5	587.4674	255.6
Dipalmitin	DG 16:0_16:0	12.67	551.5039	269.5	591.4957	264.2
Diolein	DG 18:1_18:1	12.90	603.5350	274.6	643.5282	272.7
Distearin	DG 18:0_18:0	13.97	607.5670	283.0	647.5596	278.1

Table S1: Reference data obtained from UPLC-IMS-QToF-MS measurements of diglyceride standards

Glyceride standard	Glyceride structure	Average retention time (min)	Average experimental m/z ($[M+NH_4]^+$)	Average CCS (\AA^2) ($[M+NH_4]^+$)
Tricaprilin	TG 8:0/8:0/8:0	3.54	488.3942	239.1
Tricaprin	TG 10:0/10:0/10:0	7.63	572.4883	263.9
Trilaurin	TG 12:0/12:0/12:0	13.52	656.5820	288.3
Trimyristin	TG 14:0/14:0/14:0	14.90	740.6760	312.9
Tripalmitin	TG 16:0/16:0/16:0	15.88	824.7706	335.3

Table S2: Reference data obtained from UPLC-IMS-QToF-MS measurements of triglyceride standards

CN:DB	RCOOH+NH ₃ neutral loss	
	Formula	Mass (Da)
2:0	CH ₃ COOHNH ₃	77.04768
3:0	C ₂ H ₅ COOHNH ₃	91.06333
4:0	C ₃ H ₇ COOHNH ₃	105.07898
5:0	C ₄ H ₉ COOHNH ₃	119.09463
6:0	C ₅ H ₁₁ COOHNH ₃	133.11028
7:0	C ₆ H ₁₃ COOHNH ₃	147.12593
8:0	C ₇ H ₁₅ COOHNH ₃	161.14158
9:0	C ₈ H ₁₇ COOHNH ₃	175.15723
10:0	C ₉ H ₁₉ COOHNH ₃	189.17288
12:0	C ₁₁ H ₂₃ COOHNH ₃	217.20418
13:0	C ₁₂ H ₂₅ COOHNH ₃	231.21983
14:0	C ₁₃ H ₂₇ COOHNH ₃	245.23548
14:1	C ₁₃ H ₂₅ COOHNH ₃	243.21983
15:0	C ₁₄ H ₂₉ COOHNH ₃	259.25113
15:1	C ₁₄ H ₂₇ COOHNH ₃	257.23548
16:0	C ₁₅ H ₃₁ COOHNH ₃	273.26678
16:1	C ₁₅ H ₂₉ COOHNH ₃	271.25113
16:2	C ₁₅ H ₂₇ COOHNH ₃	269.23548
17:0	C ₁₆ H ₃₃ COOHNH ₃	287.28243
17:1	C ₁₆ H ₃₁ COOHNH ₃	285.26678
17:2	C ₁₆ H ₂₉ COOHNH ₃	283.25113
18:0	C ₁₇ H ₃₅ COOHNH ₃	301.29808
18:1	C ₁₇ H ₃₃ COOHNH ₃	299.28243
18:2	C ₁₇ H ₃₁ COOHNH ₃	297.26678
18:3	C ₁₇ H ₂₉ COOHNH ₃	295.25113
18:4	C ₁₇ H ₂₇ COOHNH ₃	293.23548
19:0	C ₁₈ H ₃₇ COOHNH ₃	315.31373
19:1	C ₁₈ H ₃₅ COOHNH ₃	313.29808
19:2	C ₁₈ H ₃₃ COOHNH ₃	311.28243
20:0	C ₁₉ H ₃₉ COOHNH ₃	329.32938
20:1	C ₁₉ H ₃₇ COOHNH ₃	327.31373
20:2	C ₁₉ H ₃₅ COOHNH ₃	325.29808
20:3	C ₁₉ H ₃₃ COOHNH ₃	323.28243
20:4	C ₁₉ H ₃₁ COOHNH ₃	321.26678
20:5	C ₁₉ H ₂₉ COOHNH ₃	319.25113
20:6	C ₁₉ H ₂₇ COOHNH ₃	317.23548
21:0	C ₂₀ H ₄₁ COOHNH ₃	343.34503
21:0	C ₂₀ H ₃₉ COOHNH ₃	341.32938
21:2	C ₂₀ H ₃₇ COOHNH ₃	339.31373
22:0	C ₂₁ H ₄₃ COOHNH ₃	357.36068
22:1	C ₂₁ H ₄₁ COOHNH ₃	355.34503
22:2	C ₂₁ H ₃₉ COOHNH ₃	353.32938
22:3	C ₂₁ H ₃₇ COOHNH ₃	351.31373
22:4	C ₂₁ H ₃₅ COOHNH ₃	349.29808
22:5	C ₂₁ H ₃₃ COOHNH ₃	347.28243

22:6	$C_{21}H_{31}COOHNH_3$	345.26678
23:0	$C_{22}H_{45}COOHNH_3$	371.37633
23:1	$C_{22}H_{43}COOHNH_3$	369.36068
23:2	$C_{22}H_{41}COOHNH_3$	367.34503
24:0	$C_{23}H_{47}COOHNH_3$	385.39198
24:1	$C_{23}H_{45}COOHNH_3$	383.37633
24:2	$C_{23}H_{43}COOHNH_3$	381.36068
25:0	$C_{24}H_{49}COOHNH_3$	399.40763
25:1	$C_{24}H_{47}COOHNH_3$	397.39198
25:2	$C_{24}H_{45}COOHNH_3$	395.37633

Table S3: Calculated values of fatty acid neutral losses

ECN	CN:DB	Average retention time (mi)	Average experimental m/z ($[M+NH_4]^+$)	Average CCS (\AA^2) ($[M+NH_4]^+$)	Observed fatty acid neutral losses	Number of fingermarks [n = 30] (number of donors [n = 10])
28	TG 28:0	6.05	544.4570	255.2	8:0, 12:0	3 (2)
30	TG 30:0	7.97	572.4882	263.9	8:0, 10:0, 12:0	2 (1)
32	TG 32:0	10.56	600.5192	272.1	8:0, 12:0	6 (2)
34	TG 34:0	13.00	628.5507	278.7	6:0, 8:0, 10:0, 12:0, 14:0	6 (2)
	TG 36:1	13.13	654.5663	280.7	-	2 (1)
36	TG 36:0	13.60	656.5820	286.9	10:0, 12:0, 14:0, 16:0	12 (4)
38	TG 38:0	14.13	684.6133	293.7	10:0, 12:0, 14:0, 16:0	15 (6)
	TG 40:1	14.18	710.6287	297.5	12:0, 10:0, 18:1, 20:1	6 (2)
	TG 42:2	14.27	736.6446	302.1	14:1, 16:1	9 (5)
	TG 44:3	14.37	762.6604	307.5	14:1, 16:1	3 (1)
39	TG 43:2	14.52	750.6599	306.9	14:1, 15:0, 15:1, 16:1	3 (2)
	TG 45:3	14.58	776.6758	311.7	14:1, 15:1, 16:1	15 (8)
40	TG 40:0	14.58	712.6445	301.2	10:0, 12:0, 14:0, 16:0, 18:0	15 (5)
	TG 42:1	14.64	738.6601	306.0	12:0, 14:1, 15:0, 16:0, 16:1	30 (10)
	TG 44:2	14.72	764.6759	310.4	8:0, 12:0, 14:0, 14:1, 16:0, 16:1, 18:1	27 (9)
	TG 46:3	14.78	790.6915	315.6	14:1, 16:1	30 (10)
	TG 48:4	14.89	816.7068	321.3	-	2 (1)
	TG 40:0	14.58	712.6445	301.2	10:0, 12:0, 14:0, 16:0, 18:0	15 (5)
41	TG 41:0	14.72	726.6601	303.4	16:0	13 (8)
	TG 43:1	14.79	752.6757	309.3	12:0, 14:1, 15:0, 15:1, 16:0, 16:1	4 (4)
	TG 45:2	14.89	778.6915	314.5	13:0, 14:1, 15:0, 15:1, 16:0, 16:1, 17:1, 18:1	30 (10)
	TG 47:3	14.96	804.7071	319.2	14:1, 15:1, 16:1, 18:1	30 (10)
42	TG 42:0	14.98	740.6757	308.2	12:0, 16:0, 18:0	16 (6)

	*TG 44:1	15.03	766.6915	313.1	12:0, 14:0, 14:1, 15:0, 16:0, 16:1, 18:0	30 (10)
	*TG 46:2	15.09	792.7073	318.4	14:1, 15:0, 16:0, 16:1	30 (10)
	*TG 48:3	15.14	818.7228	323.3	14:1, 16:1	30 (10)
	TG 50:4	15.20	844.7385	329.1	-	2 (1)
	TG 54:6	15.14	896.7694	334.7	18:2	4 (2)
43	TG 43:0	15.10	754.6914	310.9	16:0	18 (7)
	*TG 45:1	15.18	780.7072	316.7	12:0, 14:0, 14:1, 15:0, 16:0, 16:1, 17:1, 18:0	26 (10)
	*TG 47:2	15.25	806.7228	322.2	14:1, 15:0, 16:1, 17:1, 18:1	30 (10)
	TG 49:3	15.29	832.7384	325.2	14:1, 15:0, 15:1, 16:1, 17:1, 18:1	30 (10)
44	TG 44:0	15.33	768.7067	315.6	12:0, 15:0, 16:0, 18:0	25 (10)
	*TG 46:1	15.38	794.7228	320.7	12:0, 14:1, 15:0, 16:0, 16:1, 18:0, 18:1	30 (10)
	*TG 48:2	15.42	820.7385	325.8	14:0, 14:1, 16:0, 16:1, 18:0, 18:1	30 (10)
	*TG 50:3	15.45	846.7541	330.7	16:1, 18:0, 18:1	30 (10)
	TG 52:4	15.45	872.7697	333.4	16:0, 18:2	4 (2)
	TG 54:5	15.43	898.7849	338.5	18:1, 18:2	11 (4)
45	TG 45:0	15.45	782.7228	318.1	18:0, 16:0	23 (9)
	*TG 47:1	15.52	808.7385	324.3	14:0, 14:1, 15:0, 16:0, 16:1, 18:0, 20:1	29 (10)
	*TG 49:2	15.56	834.7541	329.7	15:0, 16:0, 16:1, 17:1, 18:0, 18:1, 18:2	30 (10)
	TG 51:3	15.59	860.7697	334.6	16:0, 16:1, 18:1	30 (10)
	TG 53:4	15.66	886.7846	339.3	-	3 (2)
46	*TG 46:0	15.65	796.7385	322.4	14:0, 15:0, 16:0, 18:0	20 (8)
	*TG 48:1	15.69	822.7542	327.8	14:0, 16:0, 16:1, 18:0, 18:1	30 (10)
	*TG 50:2	15.72	848.7698	333.2	14:0, 16:	30 (10)

					16:1	
	*TG 52:3	15.72	874.7854	337.5	16:1, 16:0, 18:1, 18:2	30 (10)
	TG 54:4	15.71	900.8008	341.2	-	16 (6)
47	*TG 47:0	15.77	810.7541	325.8	16:0, 18:0	29 (10)
	*TG 49:1	15.81	836.7698	331.5	14:0, 15:0, 16:0, 16:1, 17:1, 18:1	30 (10)
	*TG 51:2	15.84	862.7854	336.8	14:0, 15:0, 16:0, 16:1, 17:1, 18:1, 18:2	30 (10)
	TG 53:3	15.87	888.8008	341.7	16:0, 16:1, 18:0, 18:1, 18:2, 20:0, 20:1	30 (10)
48	*TG 48:0	15.95	824.7698	329.8	16:0, 18:0, 20:0	23 (8)
	*TG 50:1	15.97	850.7854	335.5	14:0, 16:0, 16:1, 18:0, 18:1	30 (10)
	*TG 52:2	15.97	876.8009	339.9	16:0, 16:1, 18:0, 18:1	30 (10)
	TG 54:3	15.97	902.8165	344.6	18:1	28 (10)
	TG 56:4	16.08	928.8324	351.2	-	4 (2)
49	TG 49:0	16.06	838.7853	333.2	16:0, 18:0	30 (10)
	*TG 51:1	16.08	864.8010	338.7	16:0, 16:1, 18:0, 18:1	30 (10)
	TG 53:2	16.11	890.8166	343.8	16:0, 16:1, 18:0	30 (10)
	TG 55:3	16.14	916.8327	348.7	16:0, 16:1	9 (4)
50	TG 52:1	16.24	878.8165	342.1	14:0, 16:0, 18:1, 18:0,	30 (10)
	TG 54:2	16.24	904.8322	347.1	14:0, 16:0, 18:1, 18:0, 20:0	30 (10)
	TG 56:3	16.27	930.8480	351.8	14:0, 14:1, 16:0, 18:0	12 (5)
51	TG 51:0	16.32	866.8162	340.2	16:0, 18:0, 20:0	25 (9)
	TG 53:1	16.35	892.8320	345.4	14:1, 16:1, 16:0, 18:0, 20:0, 20:1	30 (10)
	TG 55:2	16.38	918.8477	350.2	14:0, 14:1, 16:0, 16:1, 18:0, 18:2, 20:0	28 (10)
52	TG 54:1	16.49	906.8476	349.1	16:0, 16:1, 18:0, 18:1, 20:0, 20:1, 22:0	30 (10)

	TG 56:2	16.50	932.8635	354.0	14:0, 14:1, 16:0, 16:1, 18:0, 18:2	28 (10)
53	TG 53:0	16.57	894.8472	347.0	14:0, 16:0	20 (8)
	TG 55:1	16.61	920.8633	352.1	12:0, 14:0, 14:1, 16:0, 16:1, 20:0, 22:0, 24:0	30 (10)
	TG 57:2	16.63	946.8790	356.9	14:0, 16:0, 16:1, 17:1	27 (10)
54	TG 54:0	16.73	908.8633	351.6	18:0	3 (3)
	TG 56:1	16.73	934.8787	355.9	14:0, 14:1, 16:0, 16:1, 18:0, 20:0	30 (10)
	TG 58:2	16.73	960.8944	360.7	14:0, 14:1, 16:0	26 (10)
55	TG 55:0	16.81	922.8783	354.6	14:0, 16:0	16 (8)
	TG 57:1	16.83	948.8944	359.3	14:0, 16:0, 16:1, 24:0	29 (10)
	TG 59:2	16.84	974.9098	364.0	14:0, 16:0, 16:1	16 (6)
56	TG 56:0	16.93	936.8945	358.4	14:0, 16:0	12 (7)
	TG 58:1	16.94	962.9101	363.1	14:0, 16:0, 16:1	29 (10)
	TG 60:2	16.95	988.9255	367.8	14:0, 14:1, 16:0	12 (7)
57	TG 57:0	17.02	950.9095	361.7	16:0, 18:0	9 (6)
	TG 59:1	17.03	976.9253	366.6	14:0, 16:0, 16:1, 18:0	14 (6)
58	TG 58:0	17.15	964.9254	365.1	14:0, 16:0, 18:0	4 (3)
	TG 60:1	17.17	990.9409	370.0	14:0, 16:0	3 (2)
59	TG 59:0	17.24	978.9412	368.8	16:0, 18:0	2 (2)

Table S4: Triglycerides identified in latent fingerprints from 10 donors. Italicised compounds are consistent with triglyceride standards. Compounds denoted with an asterisk are also presented in Table 4.