Ambient-air ozonolysis of triglycerides in aged fingerprint residues

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Supporting Information

Table S 1: HPLC gradient

RT / min	Flow rate / (mL/min)	%B
0	0.055	0
5	0.055	0
20	0.055	100
40	0.055	100
45	0.055	0
60	0.055	0

Table S 2: ESI source parameters

ESI source parameter	
Endplate Offset	500 V
Capillary Voltage	4000 V
Nebulizer	2.0 bar
Dry Gas	5 L/min
Dry Temperature	210 °C

Table S 3: Tune parameters

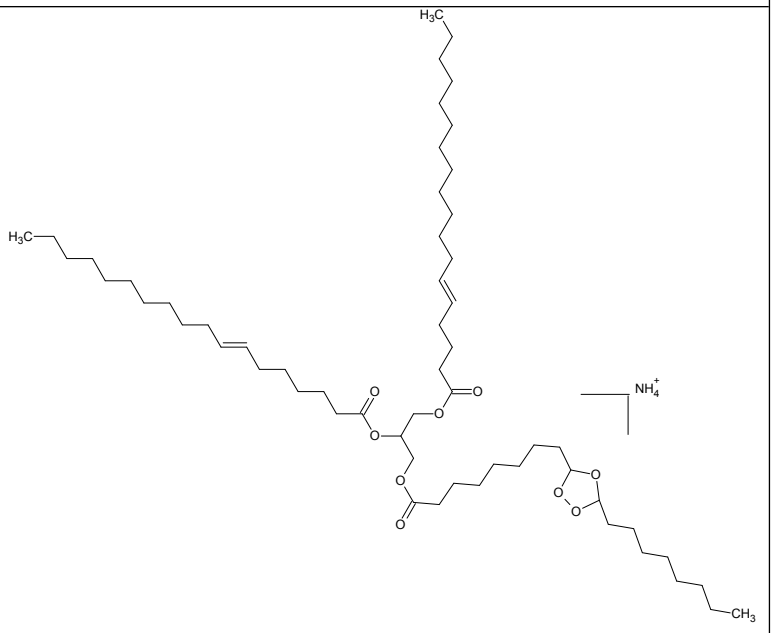
Transfer	
Funnel 1 RF	300 Vpp
Funnel 2 RF	600 Vpp
Hexapole RF	140 Vpp

Quadrupole	
Ion Energy	8 eV

Low Mass	m/z 120

Collision Cell	
Collision Energy	3 eV
Collision RF	500 Vpp
Transfer Time	80 µs
Pre Pulse Storage	10 µs

Table S 4: Proposed structures from MS^2 experiments of *m/z* 950.8019. RDB=ring double bond equivalents.

m/z	Formula	RDB	Error / ppm	Structure
950.8019	$[C_{57}H_{104}O_9]+NH_4^+$	4.5	0.042	

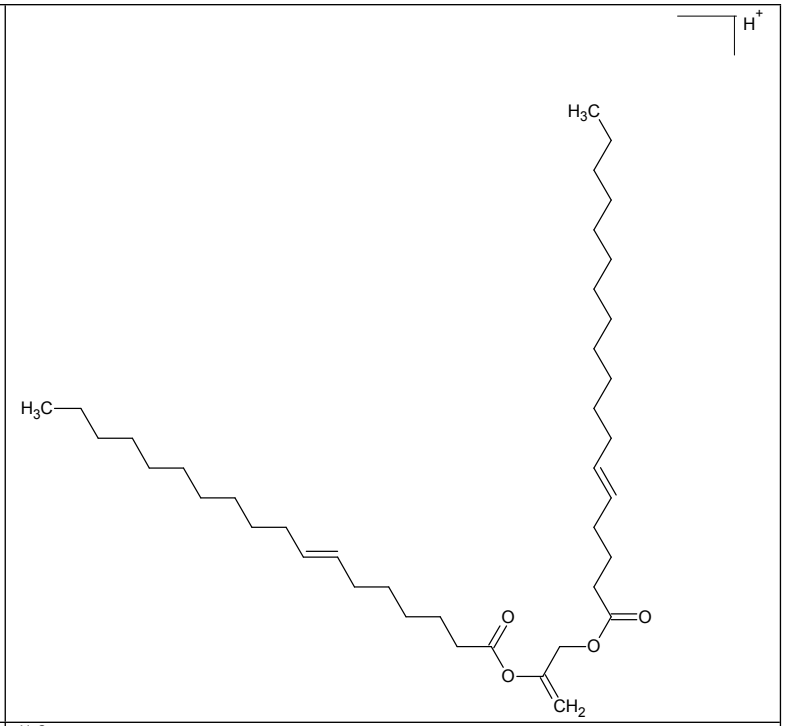
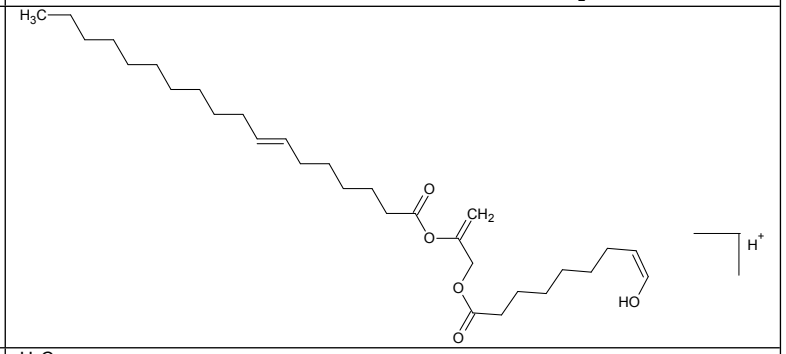
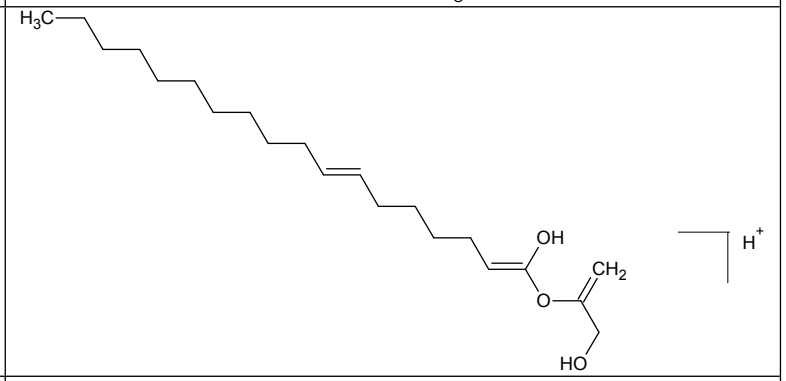
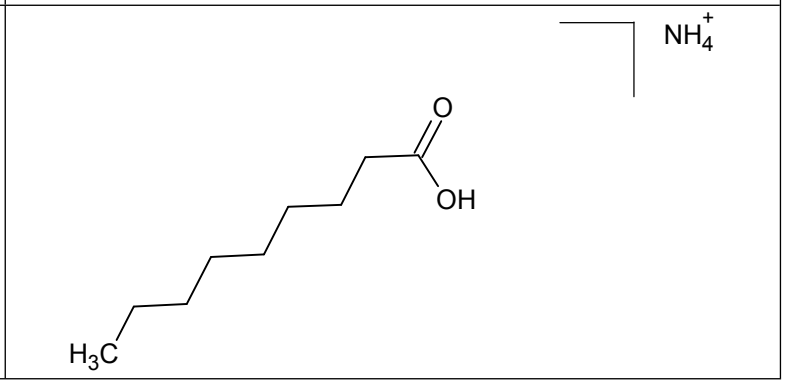
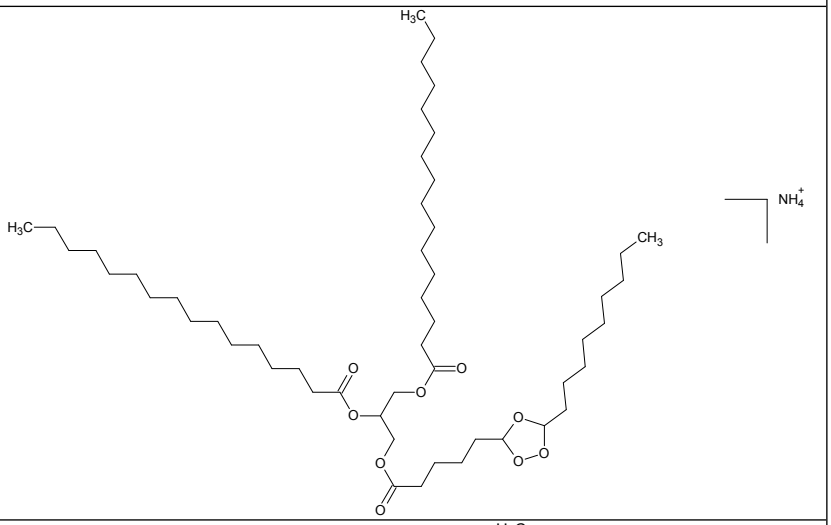
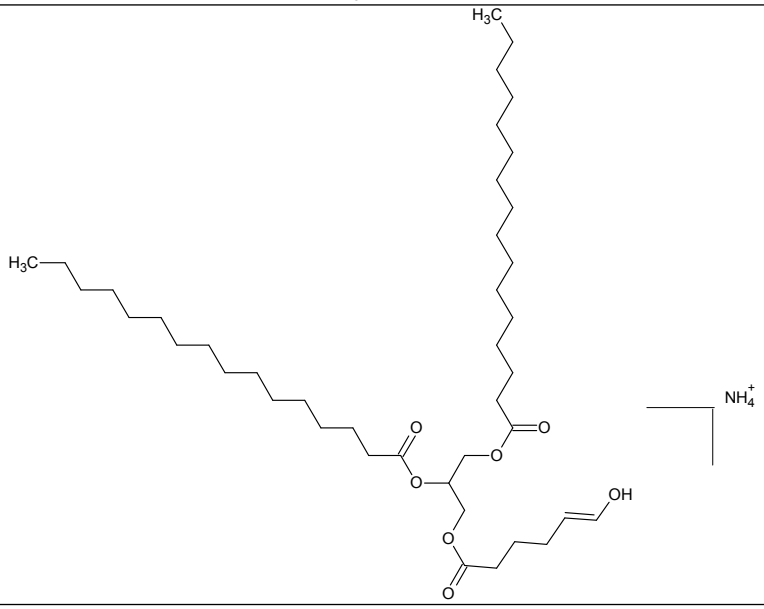
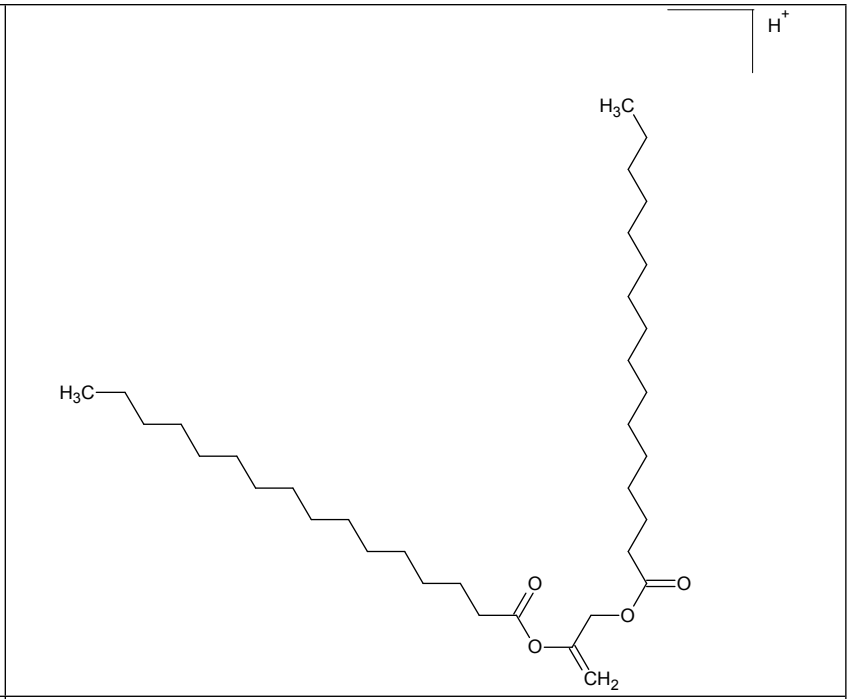
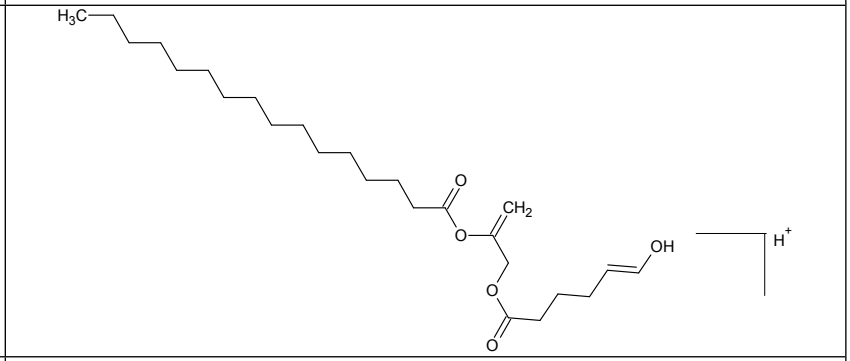
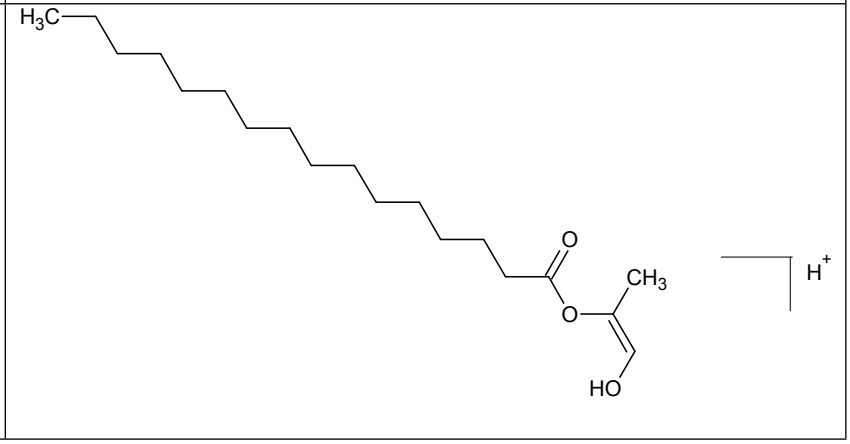
603.5338	$[C_{39}H_{70}O_4]+H^+$	4.5	-1.470	
493.3892	$[C_{30}H_{52}O_5]+H^+$	4.5	0.910	
339.2897	$[C_{21}H_{38}O_3]+H^+$	2.5	0.968	
176.1644	$[C_9H_{18}O_2]+NH_4^+$	-0.5	-0.599	

Table S 5: Proposed structures from MS² experiments of *m/z* 870.7395. RDB=ring double bond equivalents.

m/z	Formula	RDB	Error/ ppm	Structure
870.7395	$[C_{51}H_{96}O_9]+NH_4^+$	2.5	0.276	
698.5924	$[C_{41}H_{76}O_7]+NH_4^+$	2.5	-0.759	

551.5028	$[C_{35}H_{66}O_4]+H^+$	2.5	-1.064	
425.3266	$[C_{25}H_{44}O_5]+H^+$	3.5	1.056	
313.2729	$[C_{19}H_{36}O_3]+H^+$	1.5	-2.622	

190.1791	$[C_{10}H_{20}O_2]+NH_4^+$	-0.5	-5.550