

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 μ s
Pre Pulse Storage	10 μ s

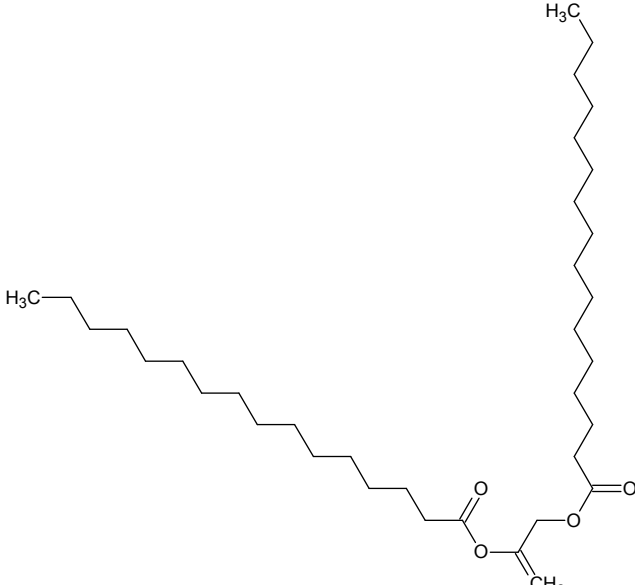
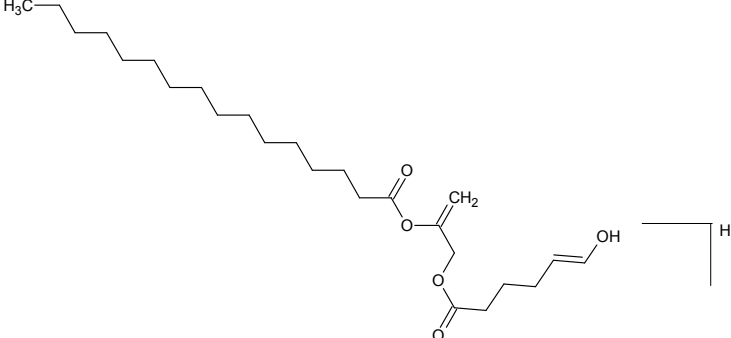
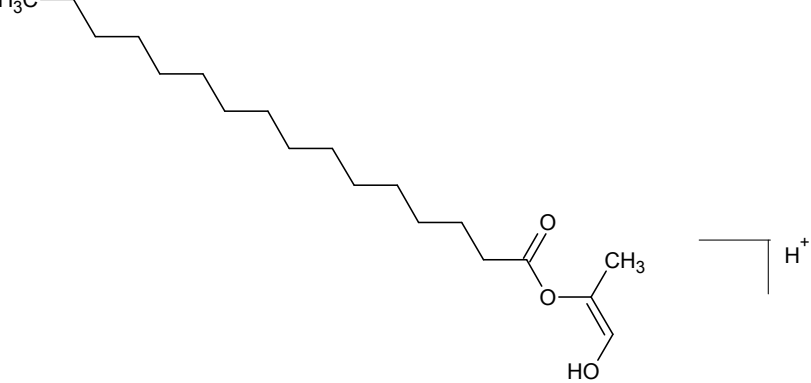
Table S 4: Proposed structures from MS² experiments of m/z 950.8019. RDB=ring double bond equivalents.

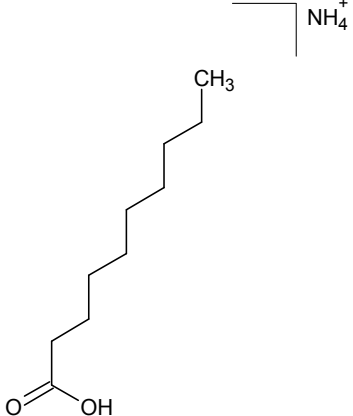
m/z	Formula	RDB	Error / ppm	Structure
950.8019	[C ₅₇ H ₁₀₄ O ₉]+NH ₄ ⁺	4.5	0.042	<p>The structure shows a long hydrocarbon chain with several double bonds and ester linkages. A terminal methyl group (H₃C) is at the top left, and another (CH₃) is at the bottom right. An ammonium ion (NH₄⁺) is shown as a separate entity to the right of the main chain.</p>

603.5338	$[C_{39}H_{70}O_4]+H^+$	4.5	-1.470	<p style="text-align: right;">H⁺</p>
493.3892	$[C_{30}H_{52}O_5]+H^+$	4.5	0.910	<p style="text-align: right;">H⁺</p>
339.2897	$[C_{21}H_{38}O_3]+H^+$	2.5	0.968	<p style="text-align: right;">H⁺</p>
176.1644	$[C_9H_{18}O_2]+NH_4^+$	-0.5	-0.599	<p style="text-align: right;">NH₄⁺</p>

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	 <p>The structure shows a long, zigzag hydrocarbon chain. At the right end, there is a methyl group (H₃C) attached to a carbon that is also bonded to a hydrogen atom. This carbon is part of a side chain that branches off from the main chain. The main chain continues to the left, ending in another methyl group (H₃C).</p>
425.3266	$[C_{25}H_{44}O_5]+H^+$	3.5	1.056	 <p>The structure features a long, zigzag hydrocarbon chain. At the right end, there is a hydroxyl group (OH) attached to a carbon that is also bonded to a hydrogen atom. This carbon is part of a side chain that branches off from the main chain. The main chain continues to the left, ending in a methyl group (H₃C).</p>
313.2729	$[C_{19}H_{36}O_3]+H^+$	1.5	-2.622	 <p>The structure shows a long, zigzag hydrocarbon chain. At the right end, there is a hydroxyl group (HO) attached to a carbon that is also bonded to a hydrogen atom. This carbon is part of a side chain that branches off from the main chain. The main chain continues to the left, ending in a methyl group (H₃C).</p>

190.1791	$[\text{C}_{10}\text{H}_{20}\text{O}_2] + \text{NH}_4^+$	-0.5	-5.550	 <p>The image shows a chemical structure of decanoic acid, represented as a zigzag chain of ten carbon atoms. The left end of the chain is a carboxylic acid group, with a double bond to an oxygen atom and a single bond to a hydroxyl group (-OH). The right end of the chain is a methyl group (-CH₃). To the right of the methyl group, there is a bracketed ammonium ion, NH₄⁺.</p>
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