Supporting Information:

Kinetics and Products from Heterogeneous Oxidation of Squalene with Ozone

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10 pages containing 6 figures and 3 talbes, showing gas-phase products from squalene oxidation (Figure S1), squalene oxidation in room air (Figure S2), mass spectrum of squalene obtained with positive mode DART-MS (Figure S3), DART-MS calibration of squalene, succinic acid and levulinic acid (Figure S4), evolution of condensed-phase products from squalene/O_3 reaction (Figure S5), DART-MS mass spectra of succinic acid and levulinic acid (Figure S6), possible products from squalene/O_3 reaction (Table S1 and S2) and m/z for mass difference (Δm/z) of 116.0 between the high molecular weight products (Table S3).

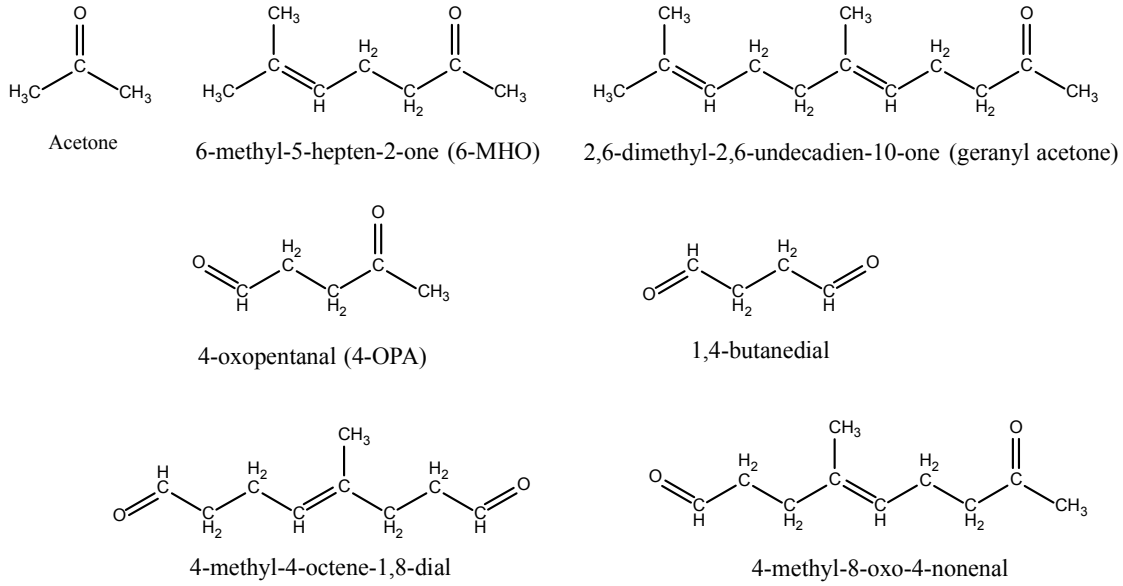


Figure S1. Gas-phase products from squalene oxidation.

Figure S2. Squalene oxidation in indoor air.

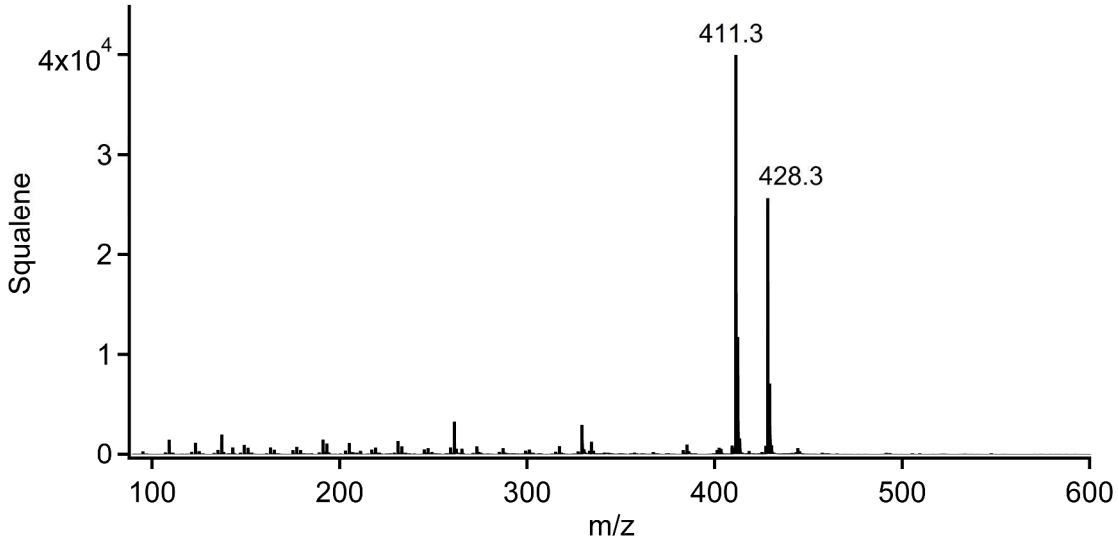


Figure S3. Mass spectrum of squalene obtained with positive mode DART-MS

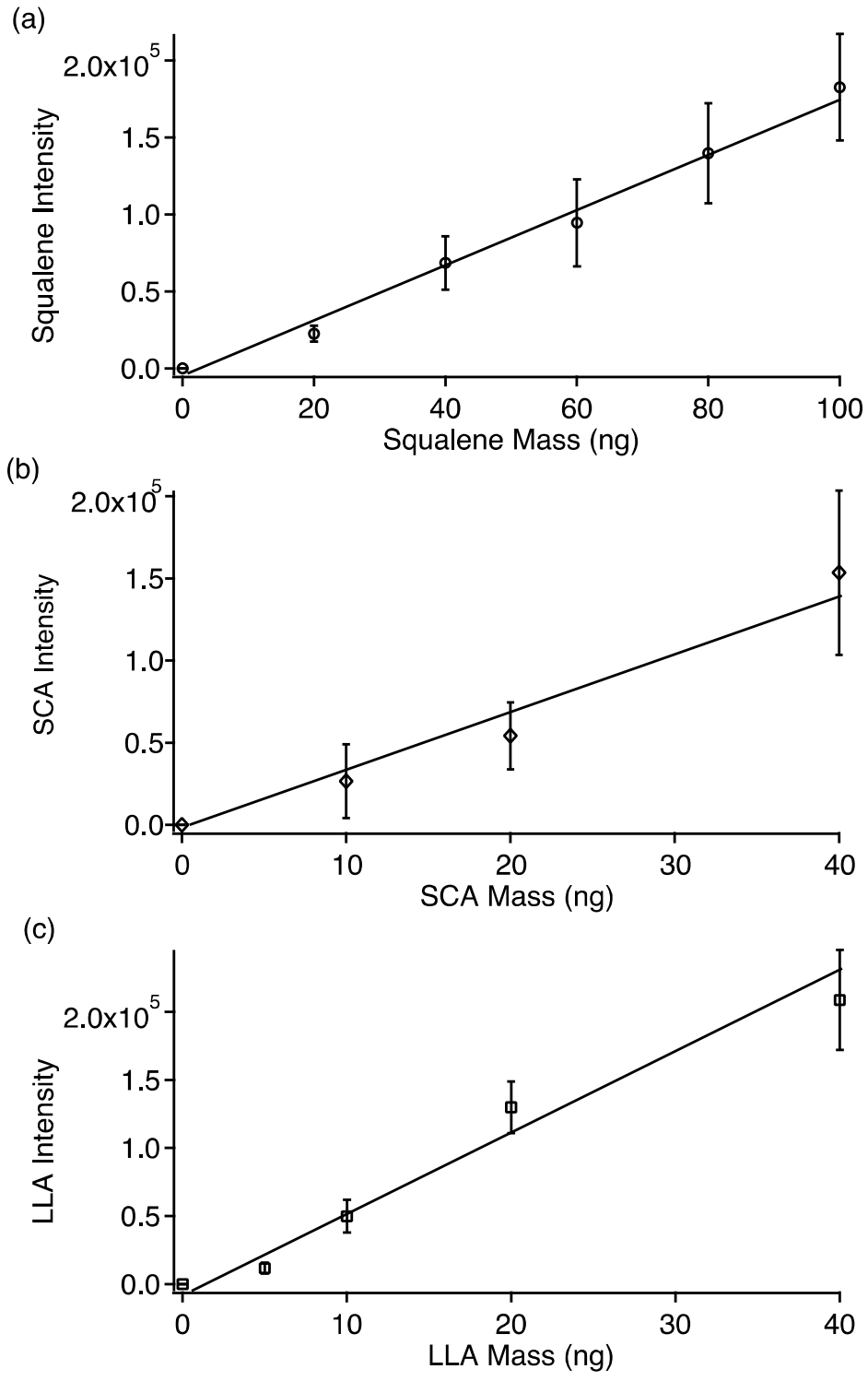


Figure S4. Calibration of (a) squalene, (b) succinic acid and (c) levulinic acid with DART-MS. Squalene was analyzed under positive mode and quantified by summing the intensities at *m/z* 411.4 and 428.4, corresponding to protonated and ammoniated squalene, respectively. Succinic and levulinic aicds were analyzed under negative mode.

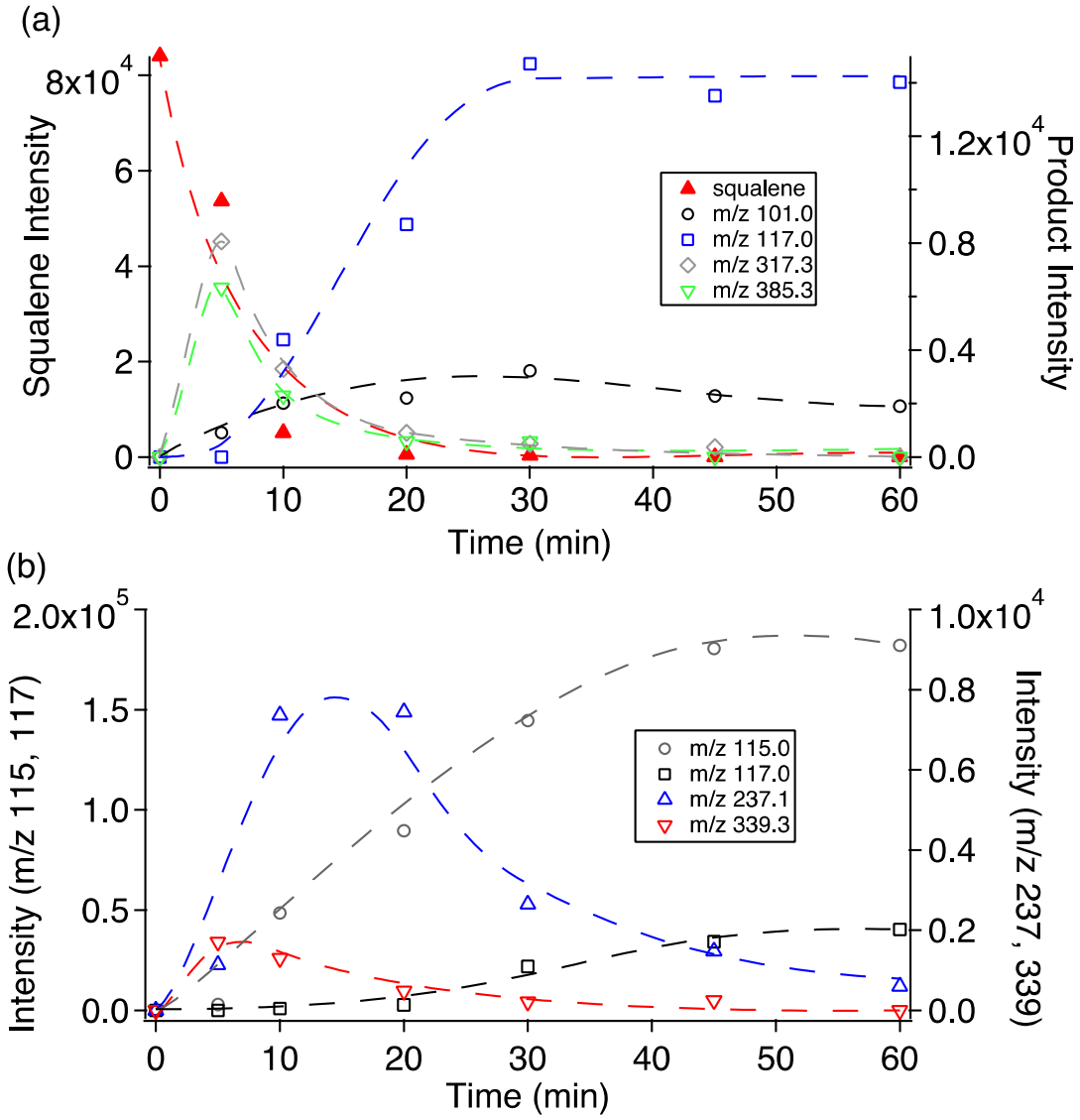


Figure S5. Evolution of the products from 50 ppb ozone reaction with 40 ng squalene obtained with (a) positive and (b) negative modes DART-MS under dry conditions. The plots show absolute intensities of reactant and products as a function of reaction time. The dashes lines are simply to guide the eye.

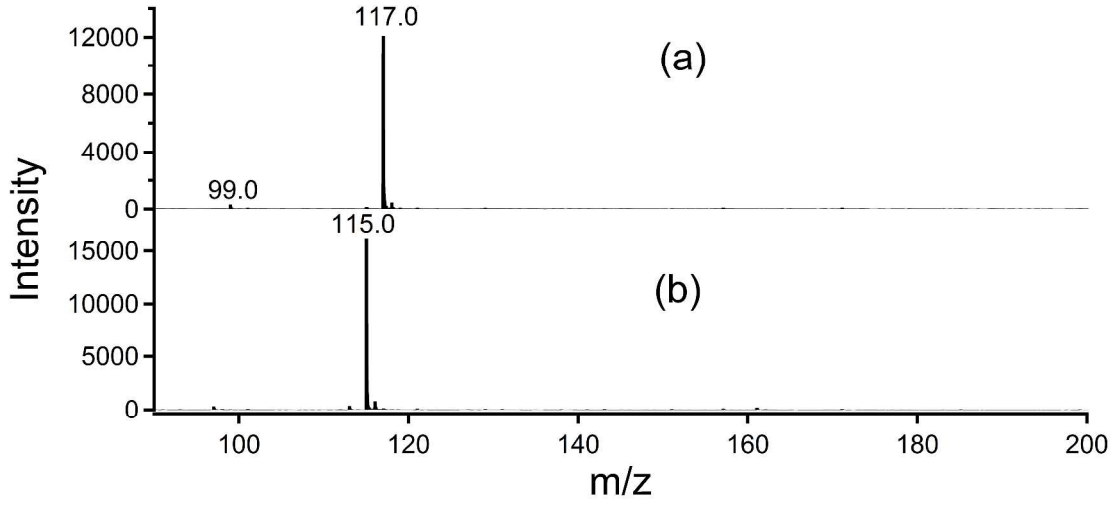


Figure S6. Mass spectra of (a) succinic acid (b) levulinic acid obtained with negative mode DART-MS.

Table S1. Possible Condensed-Phase Products Obtained with Positive Mode DART-MS from Ozone Reaction with Squalene

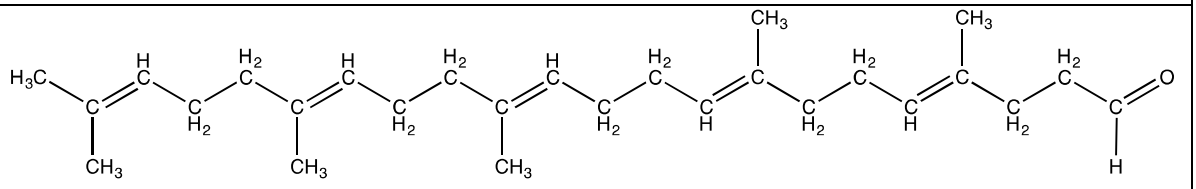
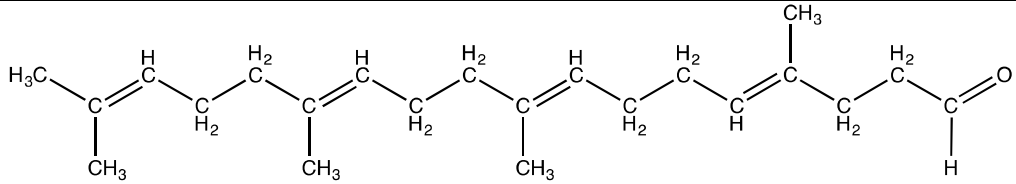
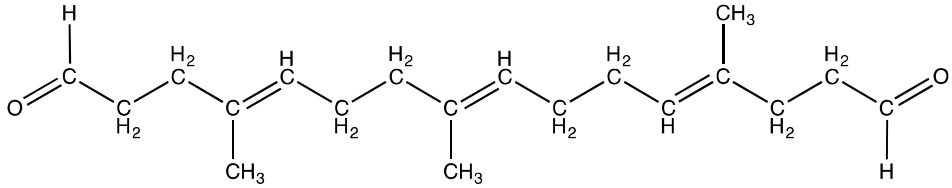
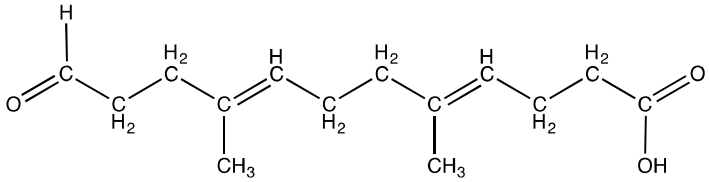
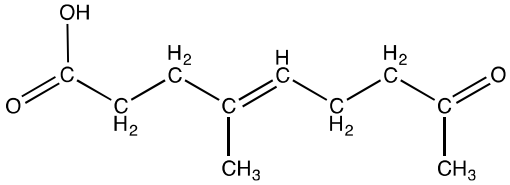
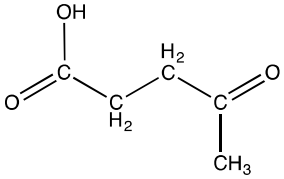
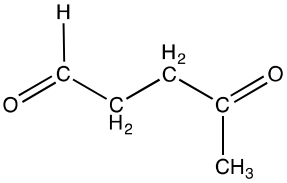
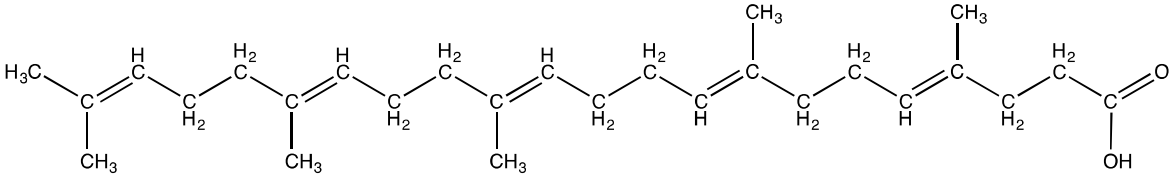
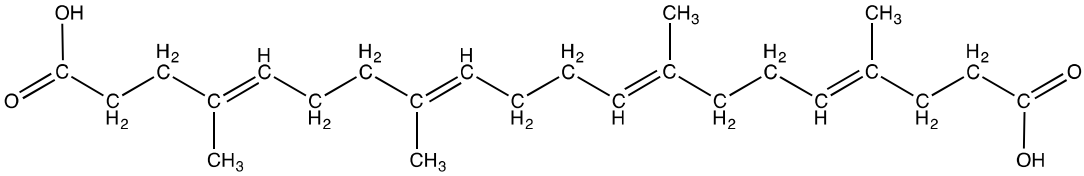
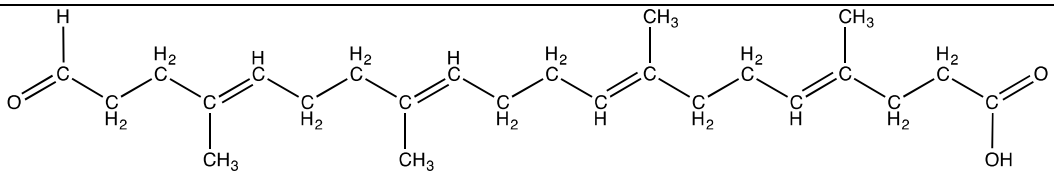
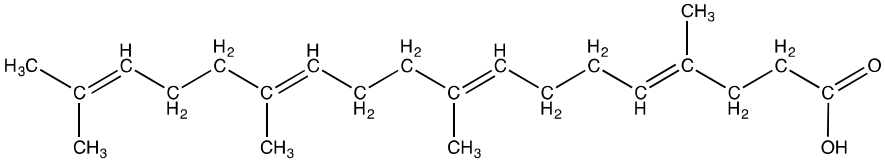
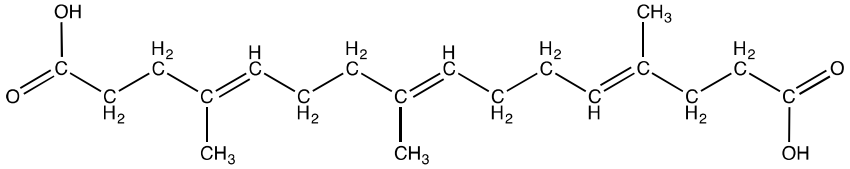
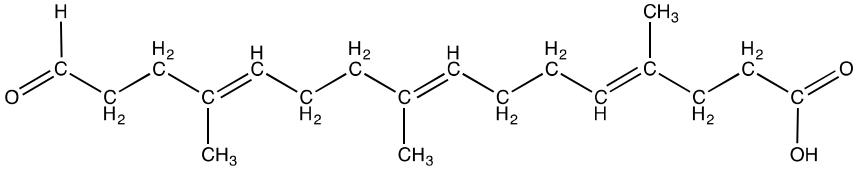
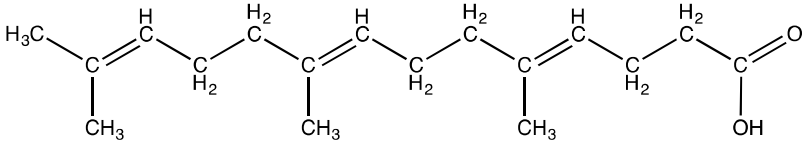
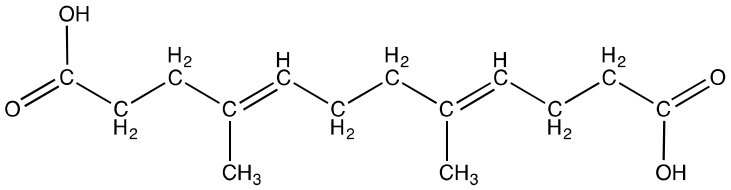
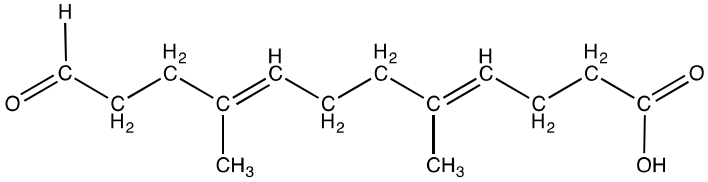
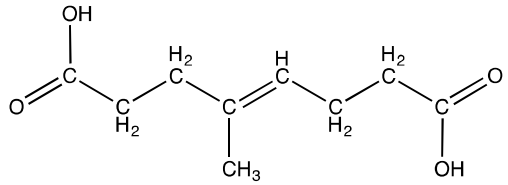
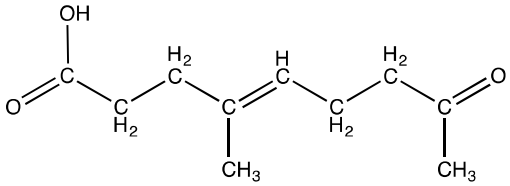
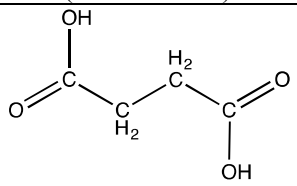
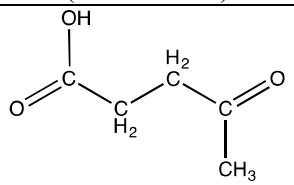
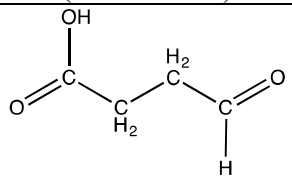
m/z	**Possible Products**
385.3	 (C27 aldehyde)
317.3	 (C22 aldehyde)
291.2	 (C19 dialdehyde)
239.1	 (C14 aldehydic acid)
185.1 (167.1)	 (C10 oxo acid)
117.0 (99.0)	 (4-oxopentanoic acid)
101.0	 (4-oxopentanal)

Table S2. Possible Condensed-Phase Products Obtained with Negative Mode DART-MS from Ozone Reaction with Squalene

m/z	**Possible Products**
399.3	 (C27 acid)
389.3	 (C24 diacid)
373.3	 (C24 aldehydic acid)
331.3	 (C22 acid)
321.2	 (C19 diacid)
305.2	 (C19 aldehydic acid)
263.2	 (C17 acid)

253.2	 (C14 diacid)
237.1	 (C14 aldehydic acid)
185.1	 (C9 diacid)
183.1	 (C10 oxo acid)
117.0	 (succinic acid)
115.0	 (levulinic acid)
101.0	 (4-oxobutanoic acid)

114
115
116
117
118

Table S3. m/z for mass difference (Δm/z) of 116.0 between the high molecular weight products

m/z	m/z+116.0	m/z+2×116.0	m/z+3×116.0
410.2	526.2	642.3	758.3
424.2	540.2	656.3	
426.2	542.2		
438.2	554.2		
440.2	556.2		
452.2	568.2	684.2	
466.2	582.2		
468.2	584.2		
482.2	598.2		
484.2	600.2	716.3	