

Supplementary Materials for
**Chemistry and human exposure implications of secondary organic aerosol
production from indoor terpene ozonolysis**

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Figs. S1 to S8
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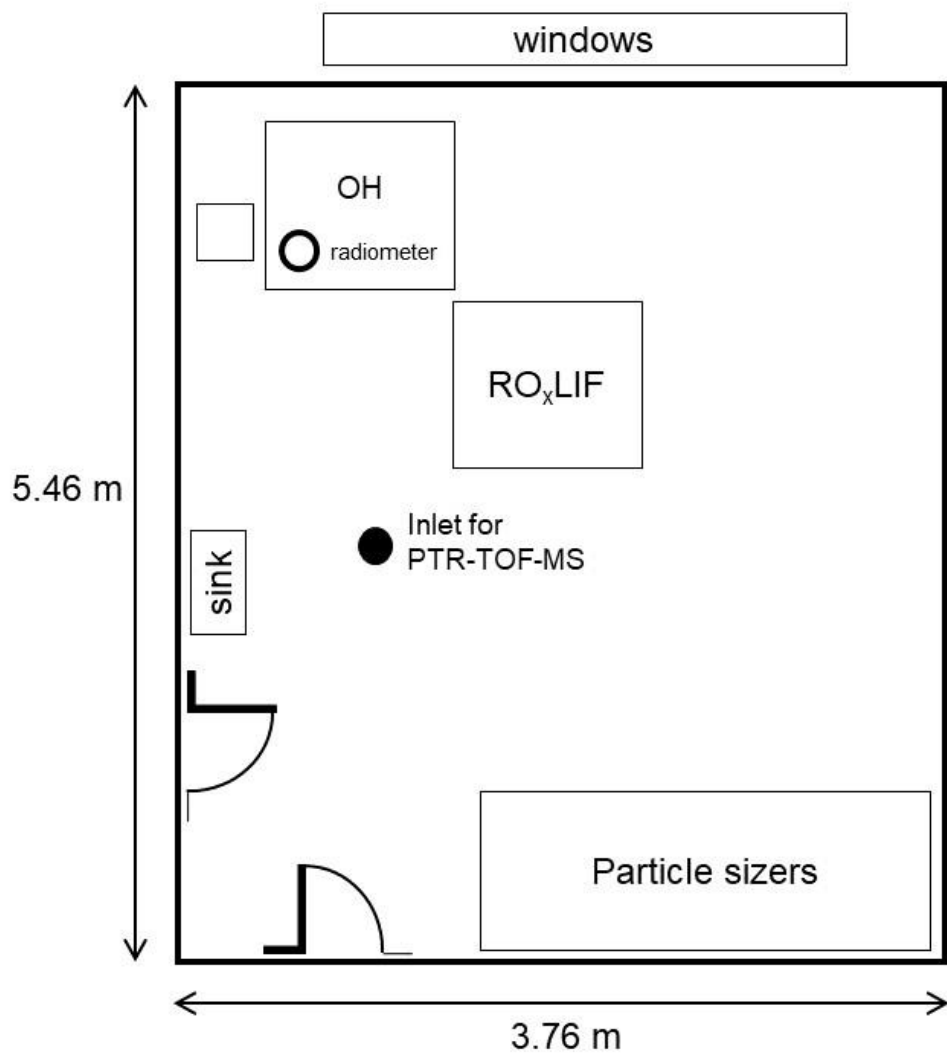


Fig. S1. Test room layout.

Spacing is approximate and instruments are not drawn to scale.

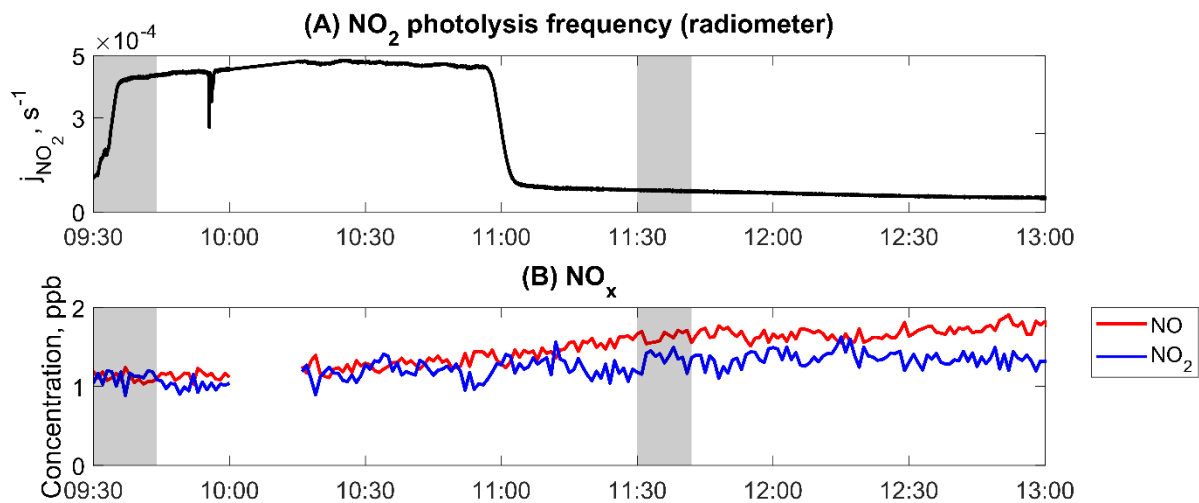


Fig. S2. Time series of additional measurements.

(A) Photolysis rate constant for NO₂ (J_{NO_2}) (B) NO_x (NO and NO₂) concentrations.

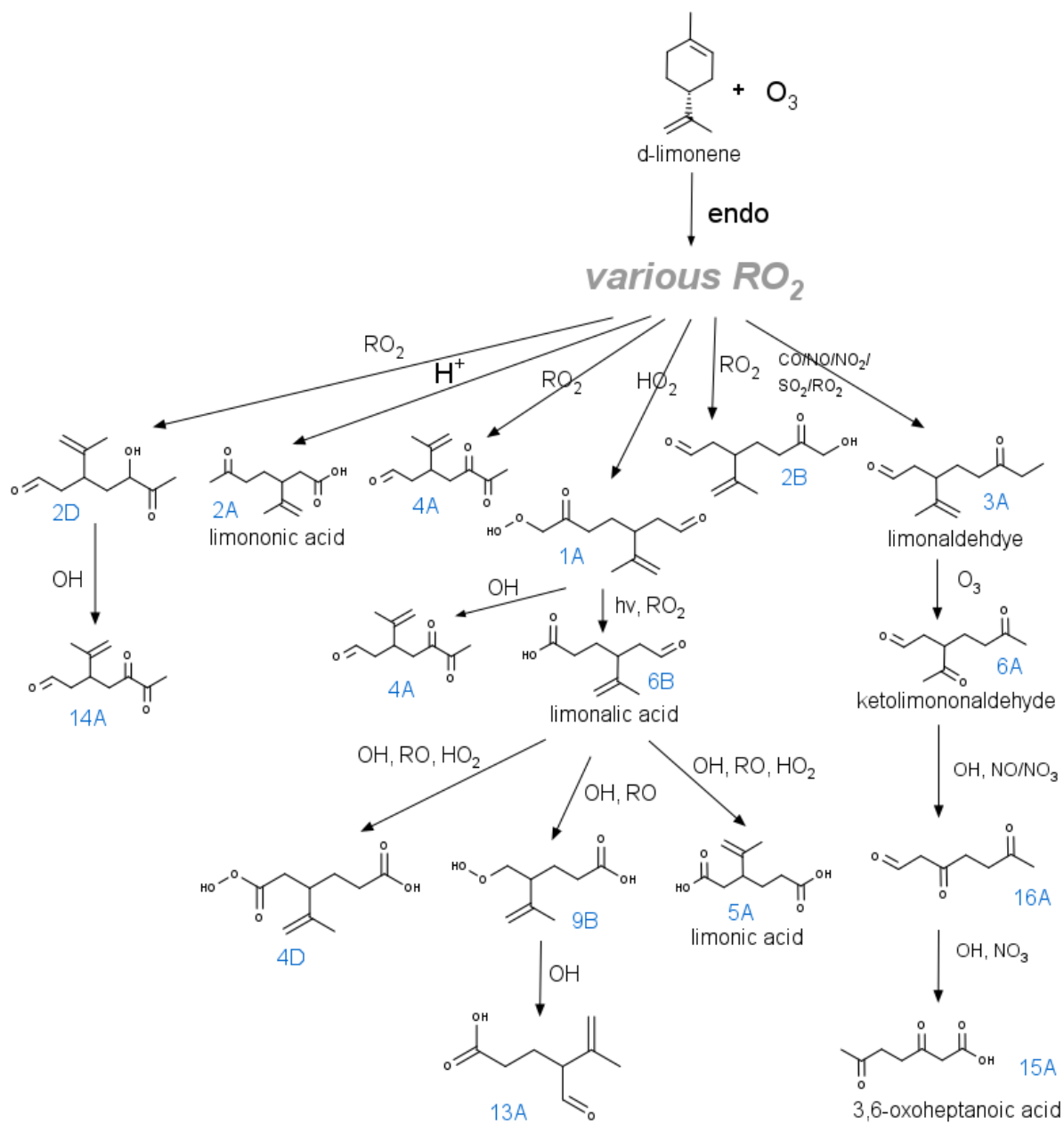


Fig. S3. Chemical mechanism for d-limonene ozonolysis through the endocyclic double bond.

The labels in blue correspond to entries in Table S2.

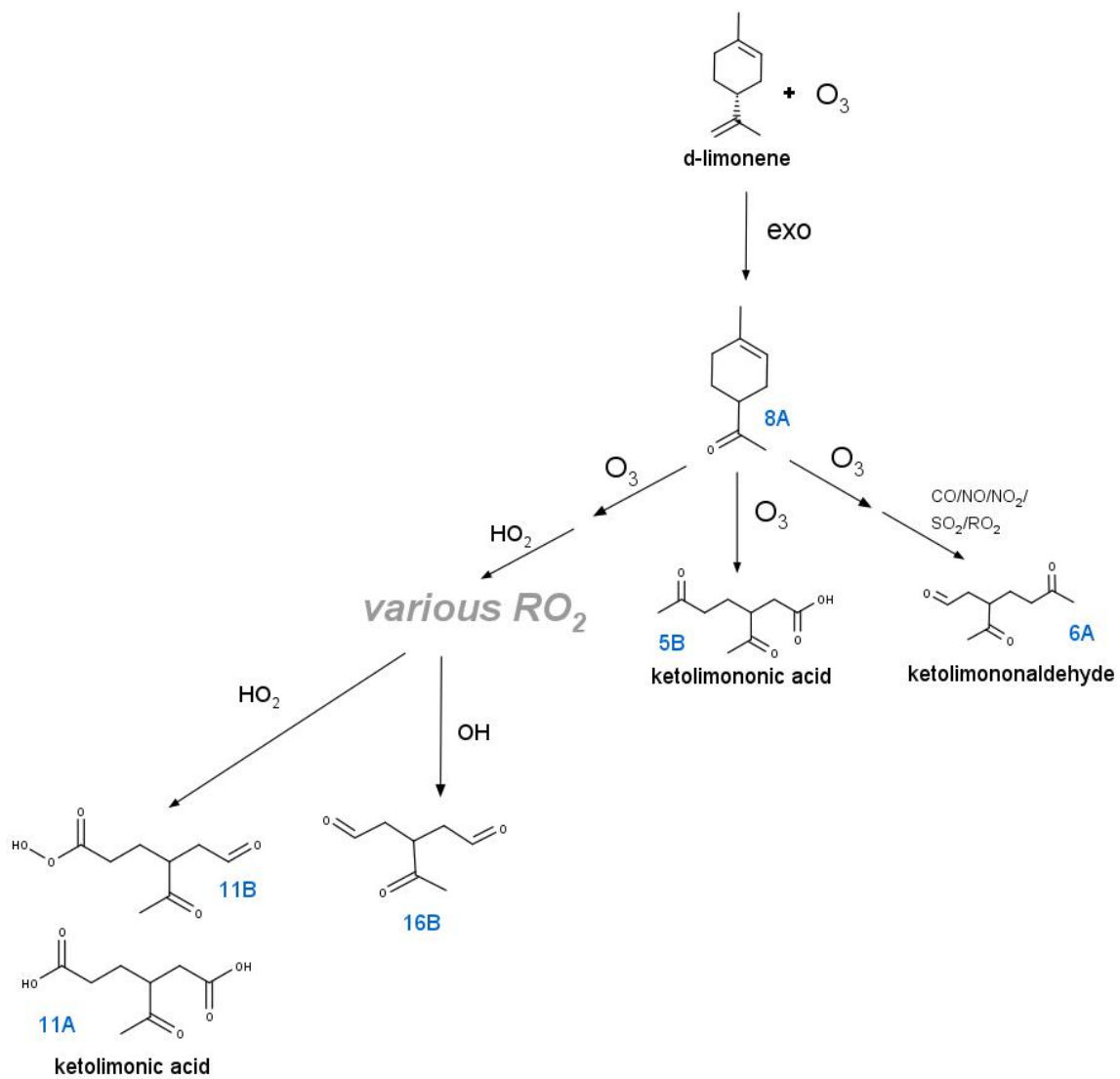


Fig. S4. Chemical mechanism for d-limonene ozonolysis through the exocyclic double bond.

The labels in blue correspond to entries in Table S2.

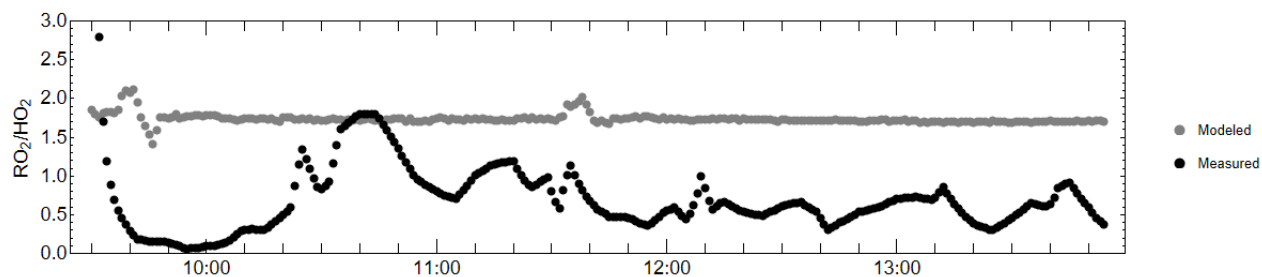


Fig. S5. RO₂-to-HO₂ ratios for measured and modeled RO₂ and HO₂.

Measured RO₂-to-HO₂ ratios range from 0.06 to 1.80, while modeled RO₂-to-HO₂ ratios range from 1.3 to 2.3. While the modeled ratios show that RO₂ is always greater than the modeled HO₂, measured ratios show that at times, measured RO₂ concentrations are at times lower than the measured HO₂ concentrations.

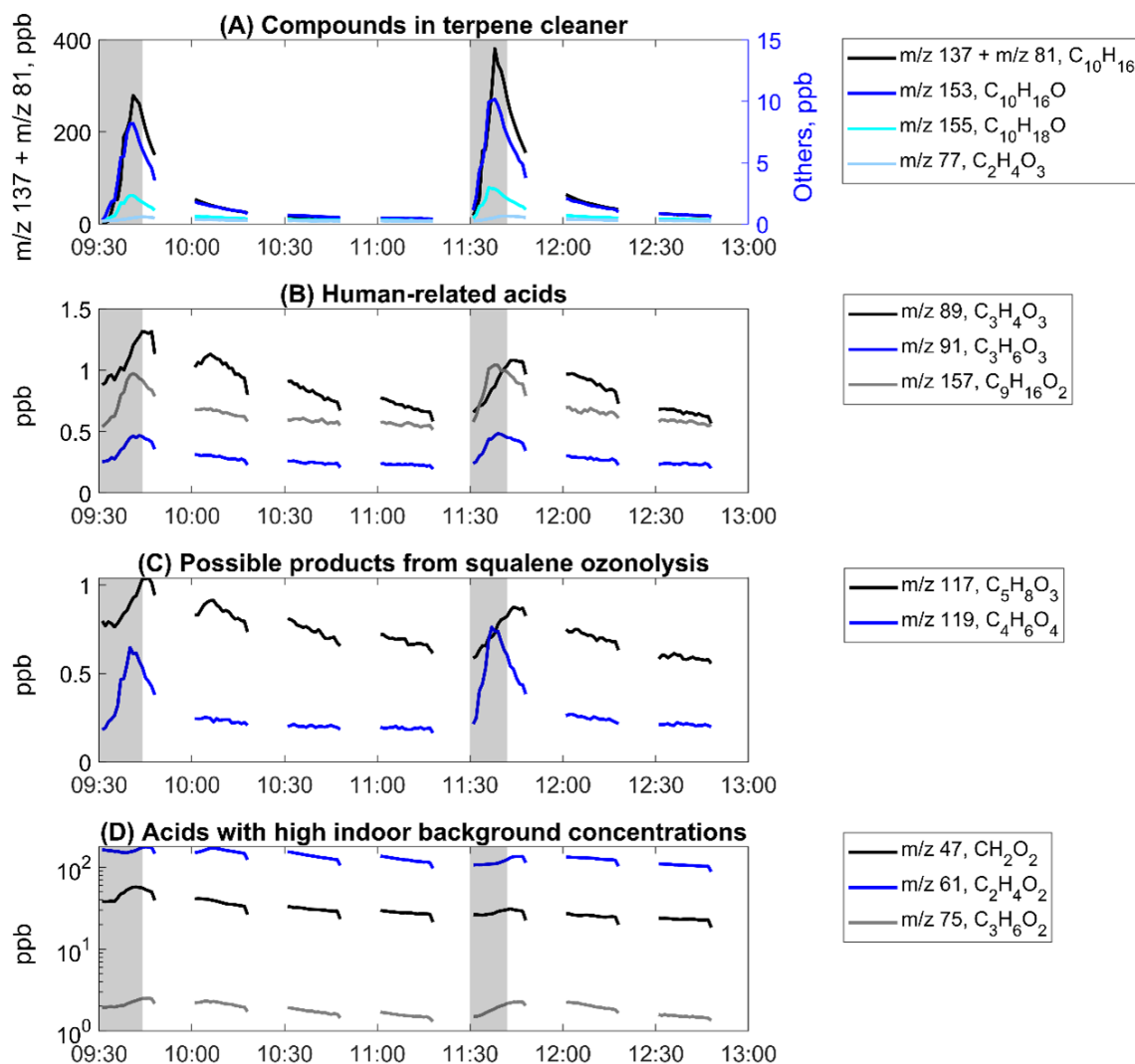


Fig. S6. Other organic compounds detected by PTR-ToF-MS.

(A) Primary emissions consumer cleaning product, (B) possible human body-associated emissions of organic acids, (C) products from squalene ozonolysis, and (D) acids with high indoor background concentrations. Gray shading corresponds to active periods of mopping and wiping during the cleaning events. Note: a researcher was present during the mopping and cleaning periods.

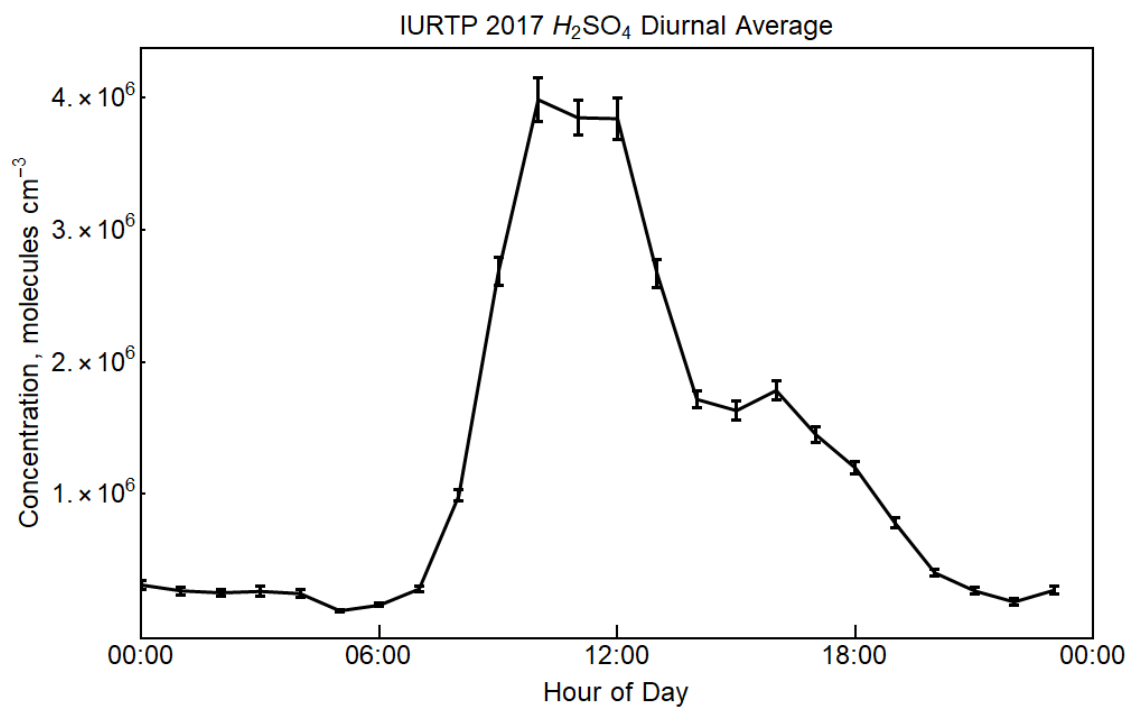


Fig. S7. Diurnal average of ambient H_2SO_4 concentrations at the IURTP field site in 2017.

Gas-phase ambient H_2SO_4 was measured with a Chemical Ionization Mass Spectrometer (CIMS) by the University of Colorado–Boulder.

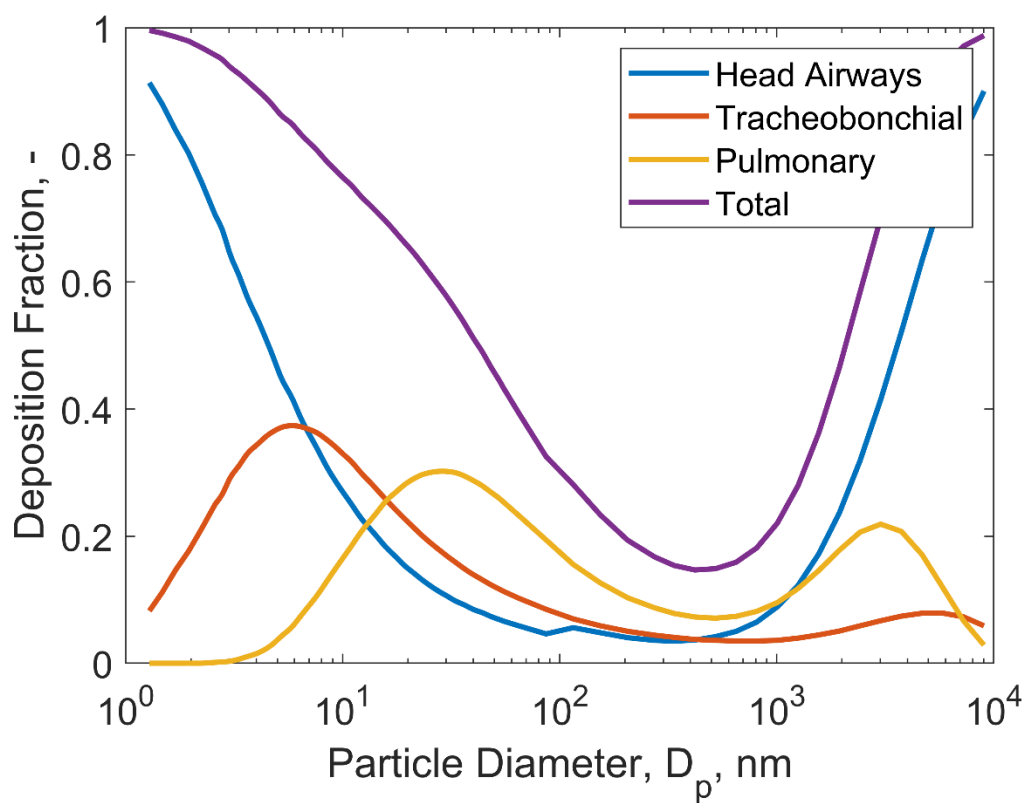


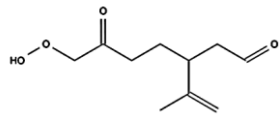
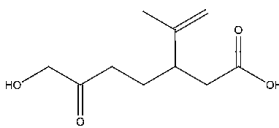
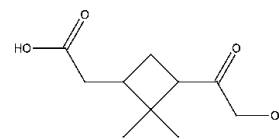
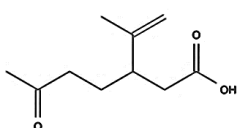
Fig. S8. Size-resolved regional and total particle deposition fractions for the human respiratory tract.

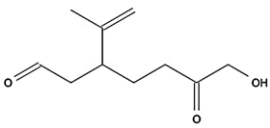
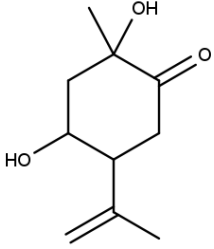
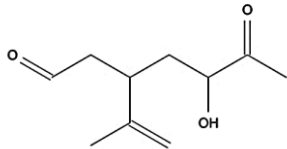
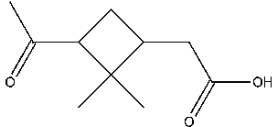
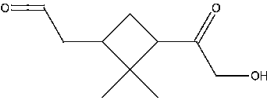
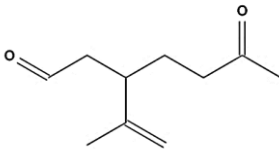
Table S1. Abundance, fraction, and ozone reaction rate constant of select monoterpenes detected via GC-MS.


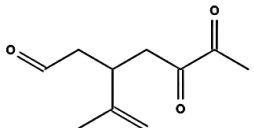
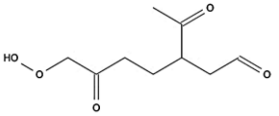
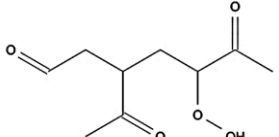
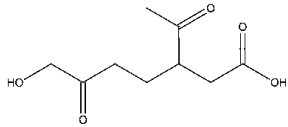
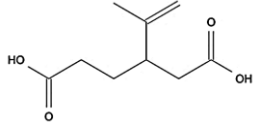
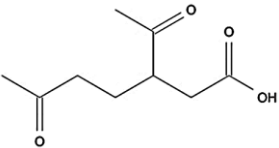
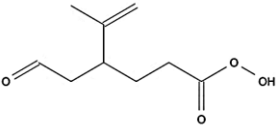
Monoterpene	Abundance (Absolute counts)	Relative fraction	Second-order rate constant ($\text{ppb}^{-1} \text{hr}^{-1}$)	Reference
d-limonene	1.1×10^7	0.44	1.9×10^{-2}	(10, 78)
α -pinene	2.5×10^6	0.10	7.56×10^{-3}	(78)
β -pinene	4.0×10^6	0.16	1.32×10^{-3}	(78)
camphene	7.5×10^6	0.30	7.94×10^{-5}	(78)

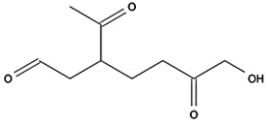
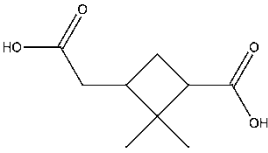
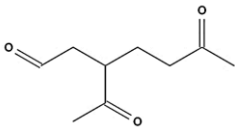
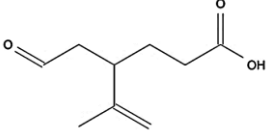
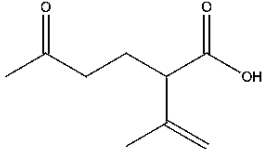
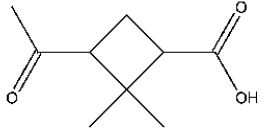
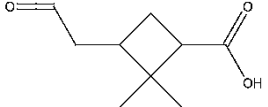
Table S2. List of gas-phase secondary oxidation products detected by PTR-ToF-MS and their molecular formula assignments.

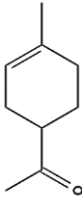
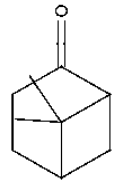
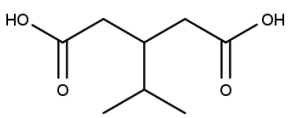
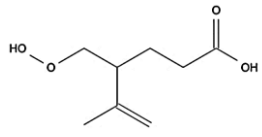
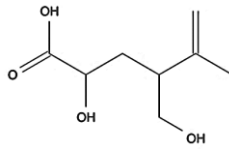
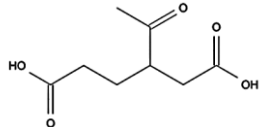
Compounds of the same molecular formula are grouped together and separated from other groups by a gray shading/border. “Label” column corresponds to the labeled structures in Figure S3 and S4, if shown. Only oxidation products from α -pinene, β -pinene, and limonene are considered.

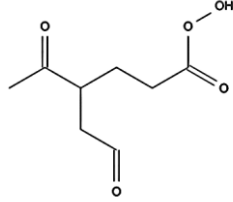
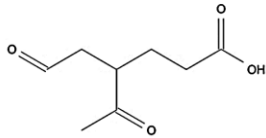
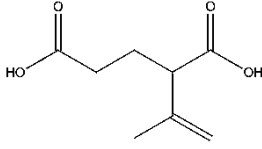
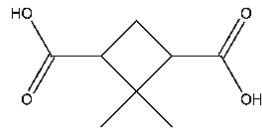
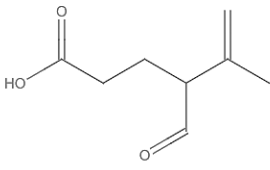
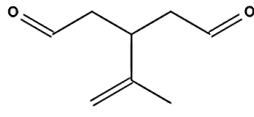
Molecular Formula	Protonated mass	Common Name (IUPAC name)	Reference	Structure	Label
$\text{C}_{10}\text{H}_{16}\text{O}_4$	201.163	-	(77, 81)		1A
		7-hydroxy-limononic acid	(82)		1B
		10-hydroxy-pinonic acid	(82)		1C
$\text{C}_{10}\text{H}_{16}\text{O}_3$	185.117221	Limononic acid (3-Isopropenyl-6-oxoheptanoic acid)	(4,82,83)		2A

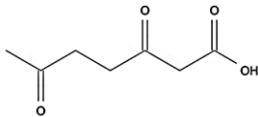
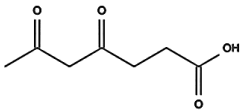
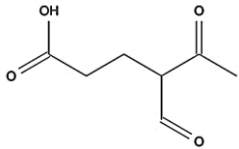
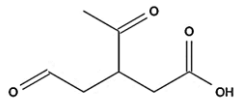
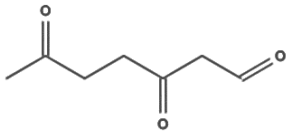
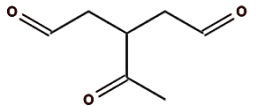
C ₁₀ H ₁₆ O ₃ (cont'd)	185.117221	7OH-lim (7-hydroxylimononaldehyde) (7-Hydroxy-3-isopropenyl-6-oxoheptanal)	(4,83)		2B
		4-Isopropenyl-1-methyl-1,5-dihydroxy-2-oxocyclohexane	(83)		2C
		-	(77,81)		2D
		Pinonic acid	(82)		2E
		10-hydroxy-pinonaldehyde	(82)		2F
C ₁₀ H ₁₆ O ₂	169.122306	Limonaldehyde/ Limonaldehyde (3-Isopropenyl-6-oxoheptanal)	(4,82)		3A

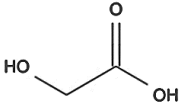
		Pinonaldehyde (2,2-dimethyl-3-acetyl-cyclobutyl-ethanal)	(77,81)		3B
C ₁₀ H ₁₄ O ₃	183.19945	(3-(2,3-Dioxobutyl)-4-methyl-4-pentalenol)	(77,81)		4A
C ₉ H ₁₄ O ₅	203.091400	-	(77,81)		4B
		-	(77,81)		4C
		7-hydroxy-keto-limononic acid	(5, 77, 81, 82)		4D
C ₉ H ₁₄ O ₄	187.096485	Limonic acid (3-Isopropenylhexanedioic acid)	(4, 5,82,83)		5A
		Keto-limononic acid (3-Acetyl-6-oxoheptanoic acid)	(5,82,83)		5B
		-	(77,81)		5C

		7-hydroxy-keto-limononaldehyde	(77, 81,82)		5D
		Pinic acid	(82)		5E
C ₉ H ₁₄ O ₃	171.101571	Keto-limononaldehyde (3-Acetyl-6-oxoheptanal)	(82,83)		6A
		Limonic acid (<i>(4R)</i> -5-Methyl-4-(2-oxoethyl)-5-hexenoic acid)	(4,5,77, 81-83)		6B
		Norlimononic acid	(5,82,83)		6C
		Norpinonic acid	(82)		6D
		Pinalic 3-acid	(82)		6E

C ₉ H ₁₄ O	139.11581	Keto-limonene/ Limonaketone (4-Acetyl-1-methyl-1-cyclohexene)	(4,77, 81, 82)		8A
		Pinaketone	(82)		8B
C ₈ H ₁₄ O ₄	175.096485	3-isopropylpentanedioic acid	(5)		9A
		-	(77,81)		9B
		-	(77,81)		9C
C ₈ H ₁₂ O ₅	189.15803	Keto-limonic acid (3-Acetylhexanedioic acid)	(5,77, 81, 82)		11A

		-	(77,81)		11B
C ₈ H ₁₂ O ₄	173.080835	Keto-limonalic acid	(5,82)		12A
		Norlimonic acid	(5,82)		12B
		Norpinic acid	(82)		12C
C ₈ H ₁₂ O ₃	157.09	-	(77,81)		13A
C ₈ H ₁₂ O ₂	141.145	-	(77,81)		14A

C ₇ H ₁₀ O ₄	159.065185	3,6-oxoheptanoic acid (3,6-Dioxoheptanoic acid)	(5,83)		15A
		4,6-oxoheptanoic acid	(5)		15B
		(4-Formyl-5-oxohexanoic acid)	(77, 81)		15C
		(4-Oxo-3-(2-oxoethyl)pentanoic acid)	(77, 81)		15D
C ₇ H ₁₀ O ₃	143.135	-	(77, 81)		16A
		-	(77, 81)		16B

$C_2H_4O_3$	77.023320	Glycolic acid	(77)		17
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