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Supplementary Information for

Aqueous-phase fates of α-alkoxyalkyl-hydroperoxides derived from the reactions of Criegee intermediates with alcohols

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No. of Supporting Pages: 10

No. of Supporting Tables: 1

No. of Supporting Figures: 9

Table S1. Rate Coefficients and Lifetimes for Decay of the α-HHs derived from α-Terpineol Ozonolysis in 1-propanol:Water Solutions at Different pH. $\tau_{1/e} = 1/k_{fast}$.

[HCl] (mM)	pH	k_{fast} (10^{-3} s^{-1})	k_{slow} (10^{-3} s^{-1})	$\tau_{1/e,\ decay}$ (min)
0.01	5.3	1.0 ± 0.1	0.14 ± 0.03	17
0.02	4.9	1.4 ± 0.1	0.28 ± 0.02	12
0.05	4.5	2.0 ± 0.3	0.19 ± 0.01	8
0.1	4.0	3.1 ± 0.6	0.10 ± 0.04	5
0.2	3.8	5.6 ± 0.5	0.10 ± 0.03	3

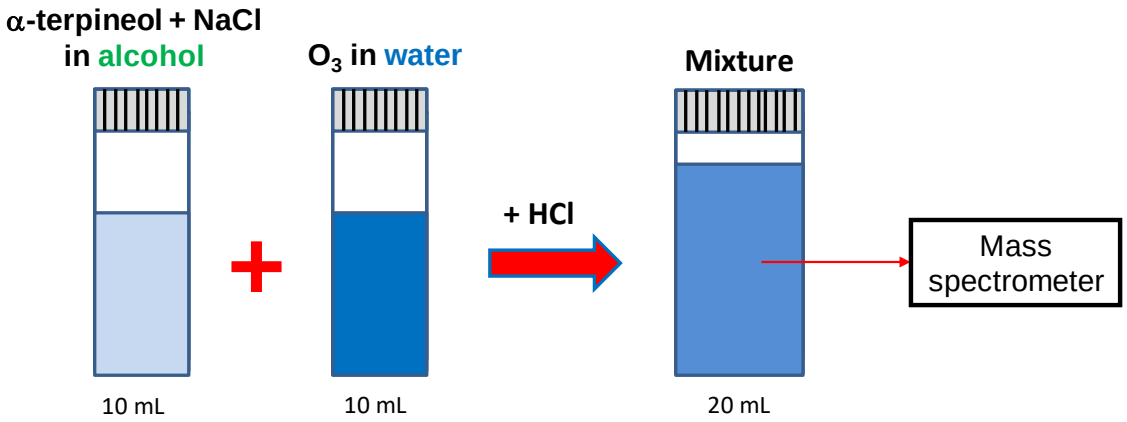

Figure S1 – Schematic setup of present experiment.

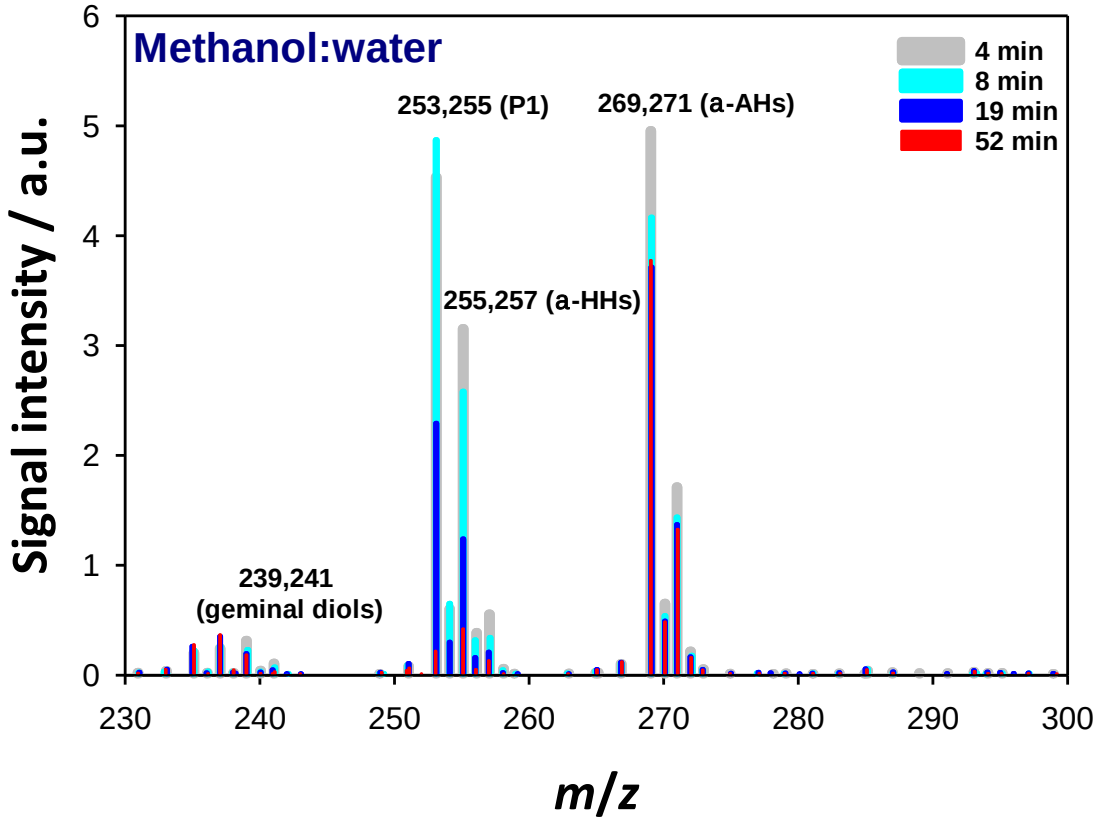

Fig. S2. Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of aqueous solutions of α-terpineol (1 mM), NaCl (0.2 mM) in methanol:H_2O (1:1 = vol:vol) solution at T = 298 K. 0.05 mM HCl was added to the solution.

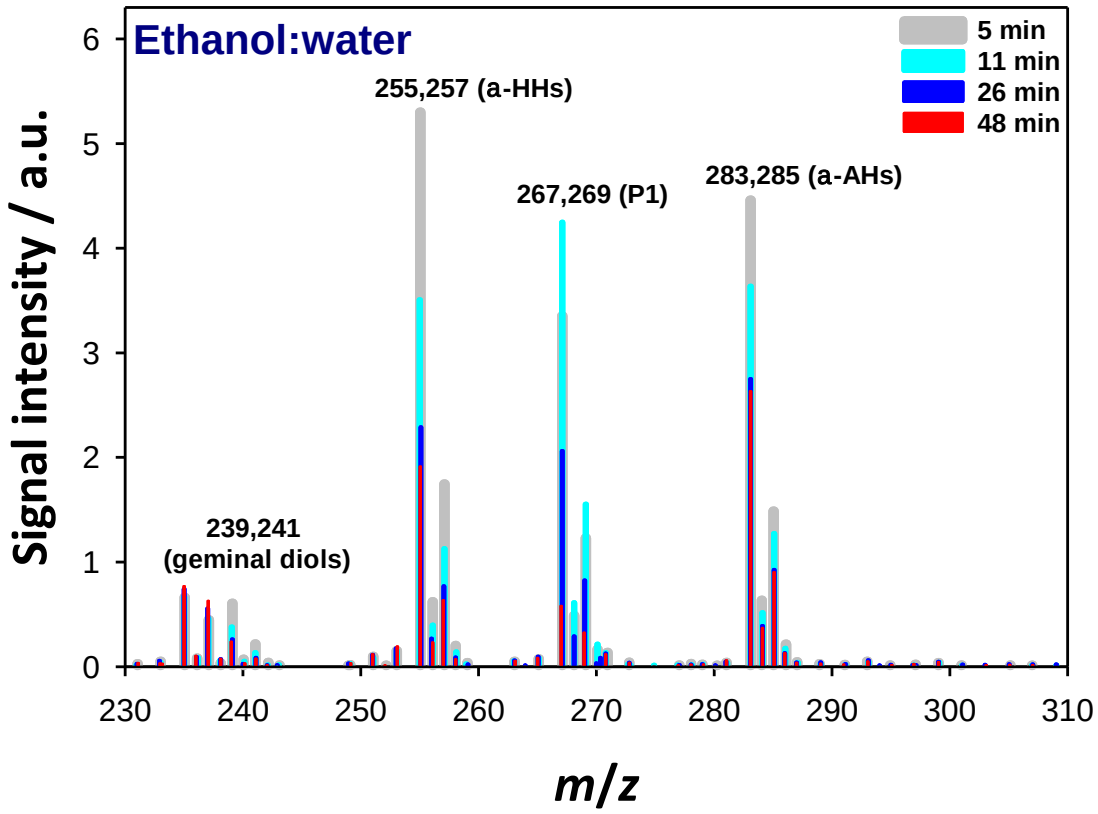

Fig. S3. Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 $\pm$ 0.01 mM) of aqueous solutions of α-terpineol (1 mM), NaCl (0.2 mM) in ethanol:H_2O (1:1 = vol:vol) solution at T = 298 K. 0.05 mM HCl was added to the solution.

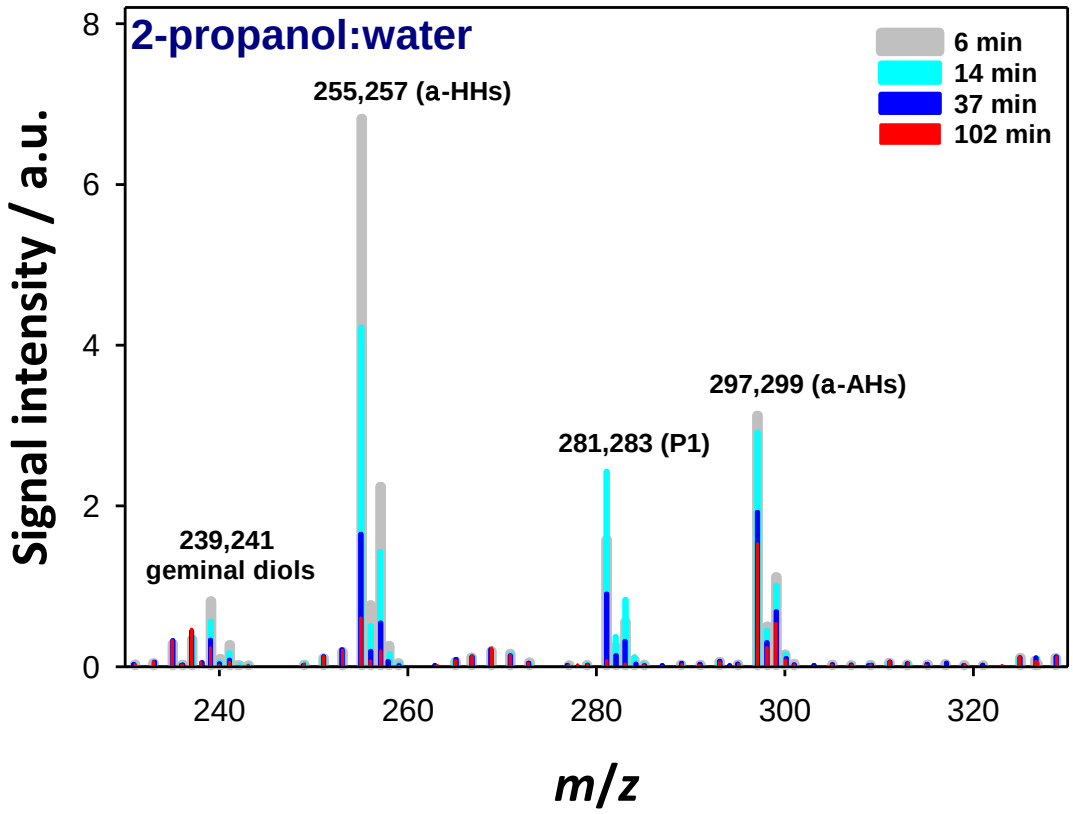

Fig. S4. Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of aqueous solutions of α-terpineol (1 mM), NaCl (0.2 mM) in 2-propanol:H_2O (1:1 = vol:vol) solution at T = 298 K. 0.05 mM HCl was added to the solution.

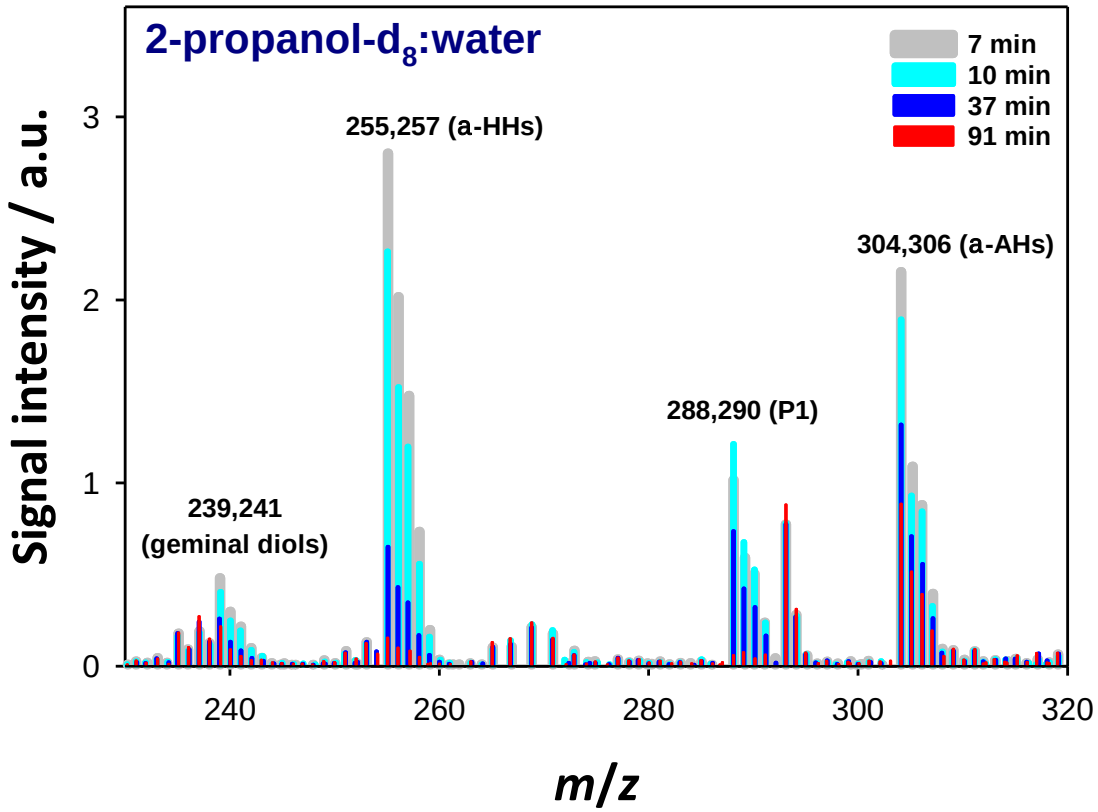

Fig. S5. Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of aqueous solutions of α-terpineol (1 mM), NaCl (0.2 mM) in 2-propanol-d_8:H_2O (1:1 = vol:vol) solution at T = 298 K. 0.05 mM HCl was added to the solution. Note that the α-AH signals appearing at *m/z* = 154 (α-terpineol) + 48 (O_3) + 68 (2-propanol-d_8) + 35/37 (Cl^-) = 305/307 was shifted to – 1 Da due the exchange of hydroperoxide -OO-D by -OO-H from H_2O.

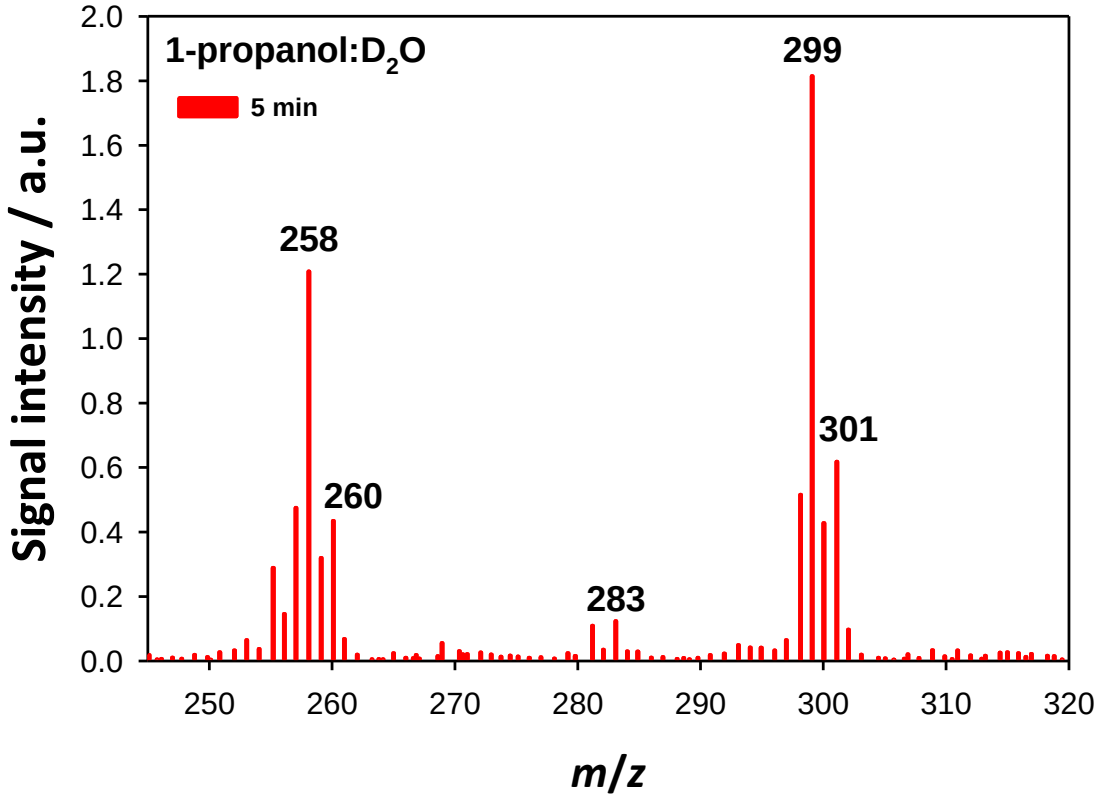

Fig. S6. Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of aqueous solutions of α-terpineol (1 mM), NaCl (0.2 mM) in 1-propanol:D_2O (1:1 = vol:vol) solution at T = 298 K. 0.05 mM HCl was added to the solution.

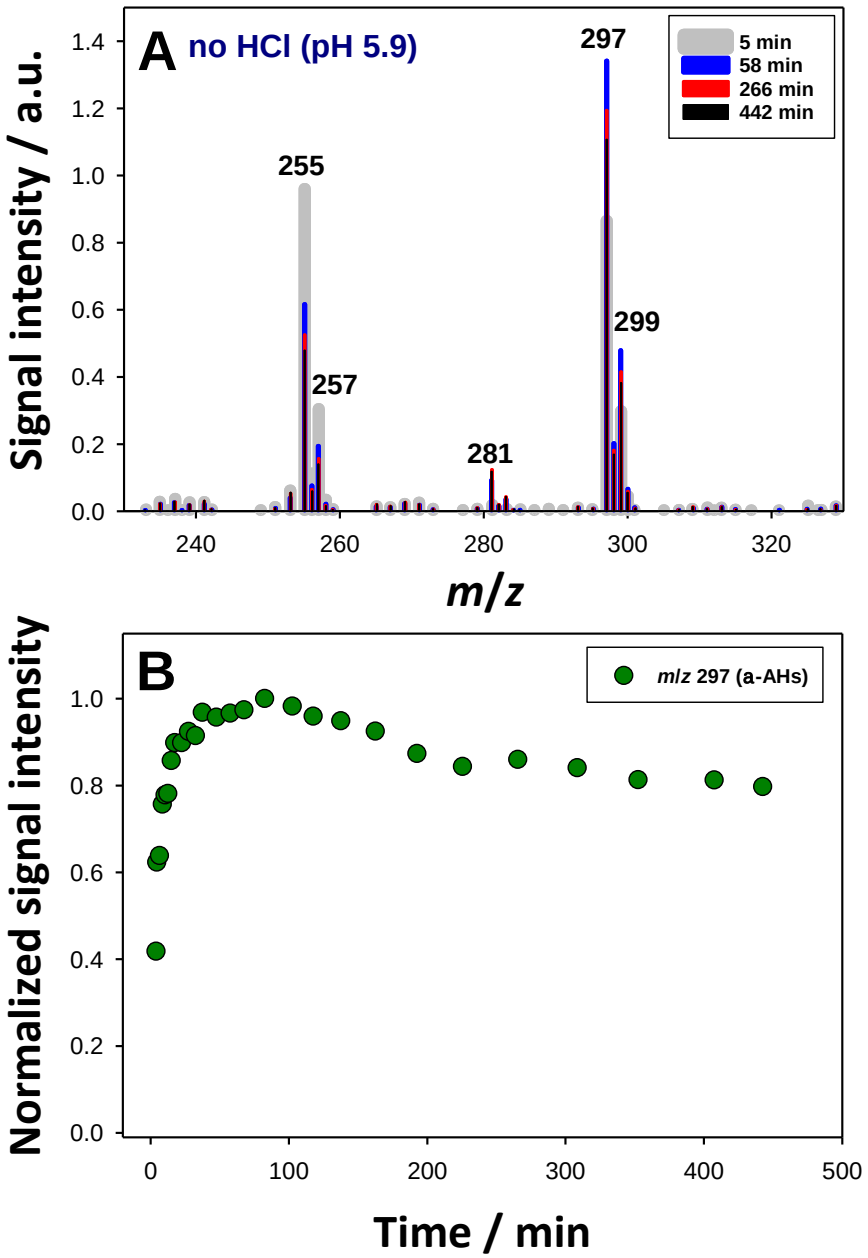

Fig. S7. A)Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of aqueous solutions of α-terpineol (1 mM), NaCl (0.2 mM) in 1-propanol:H_2O (1:1 = vol:vol) solution in the absence of HCl at pH 5.9 and at T = 298 K. B) Normalized signal intensity at m/z 297 as a function of time.

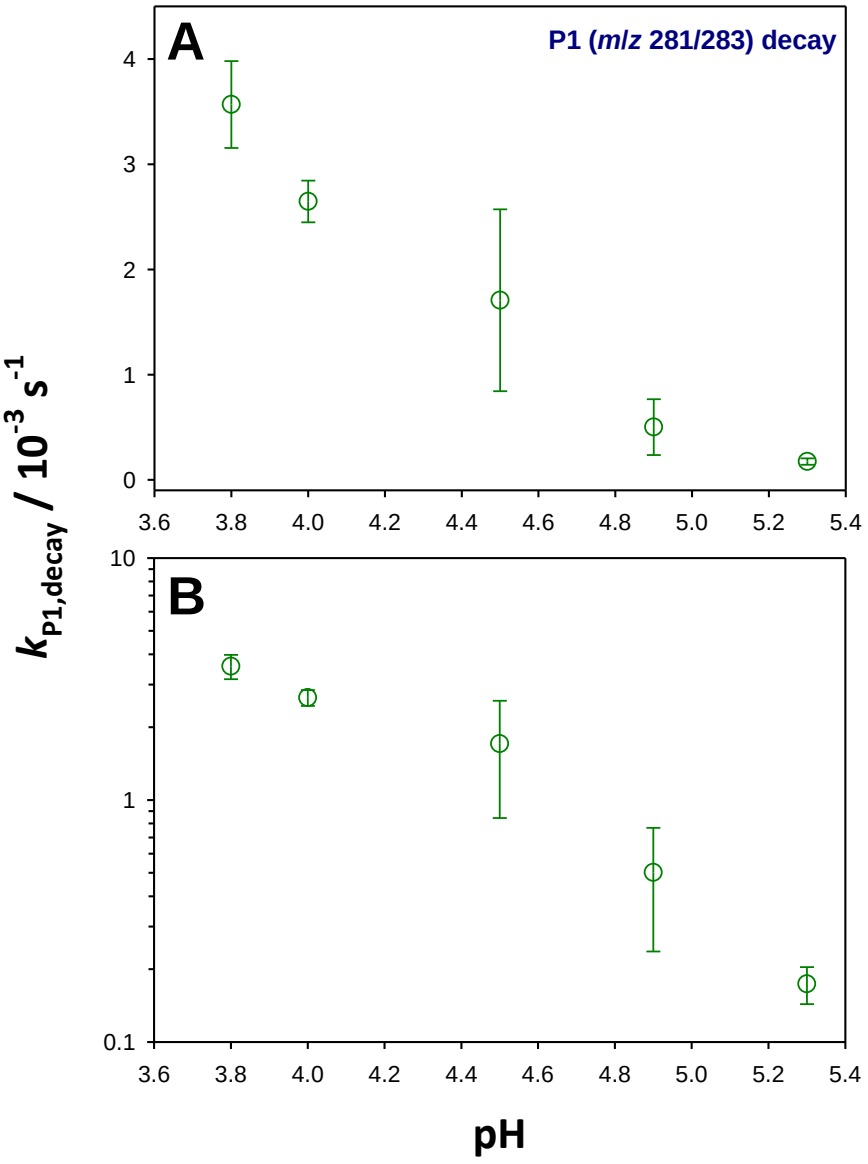

Fig. S8. A) The rate coefficients *k* for the decay of the *m*/*z* 281/283 signals obtained by ozonolysis of α-terpineol (1 mM α-terpineol, 0.2 mM NaCl) at $[O_3]_0$ = 0.06 ± 0.01 mM in 1-propanol:water (1:1 = vol:vol) solution as a function of pH at T = 298 K. B) The semi-log plot.

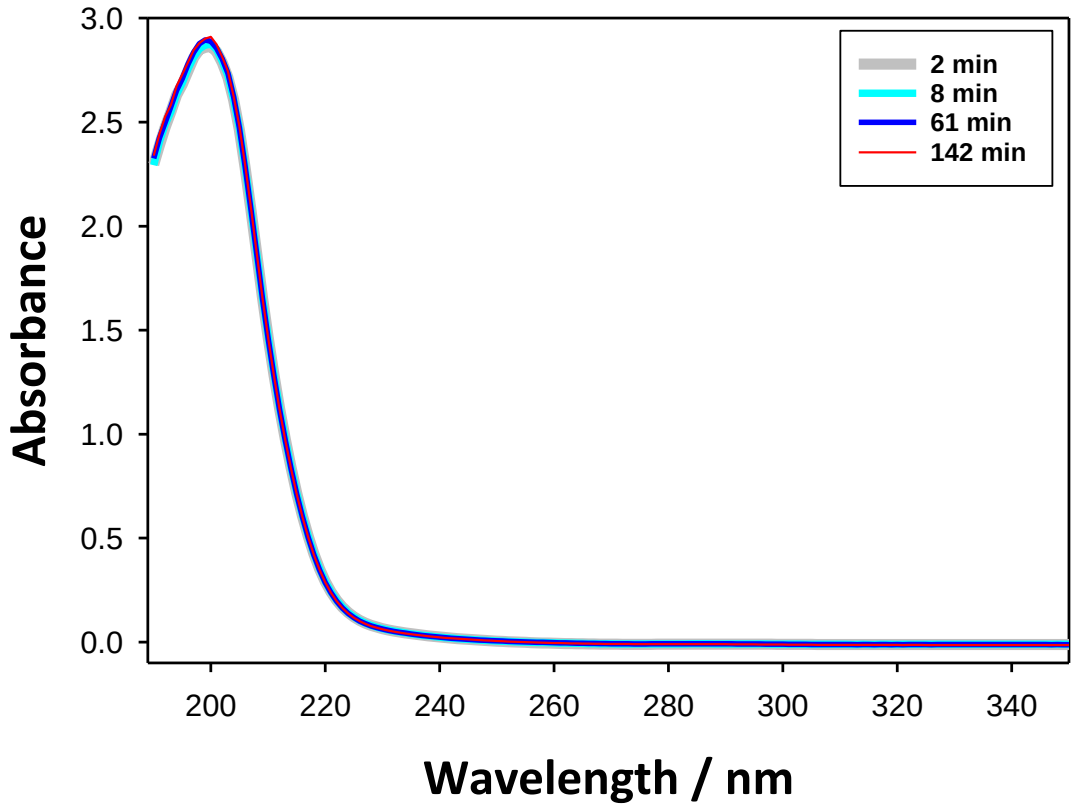

Fig. S9. UV-vis spectra obtained from 1 mM α-terpineol + 0.2 mM NaCl + 0.06 mM O_3 in 1-propanol:water (1:1) solution at pH 4.5 (by adding 0.05 mM HCl) after ozonolysis as a function of reaction time.