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Supplementary Information for

Decomposition of multifunctionalized α-alkoxyalkyl-hydroperoxides derived from the reactions of Criegee intermediates with diols in liquid phases

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No. of Supporting Figures: 7

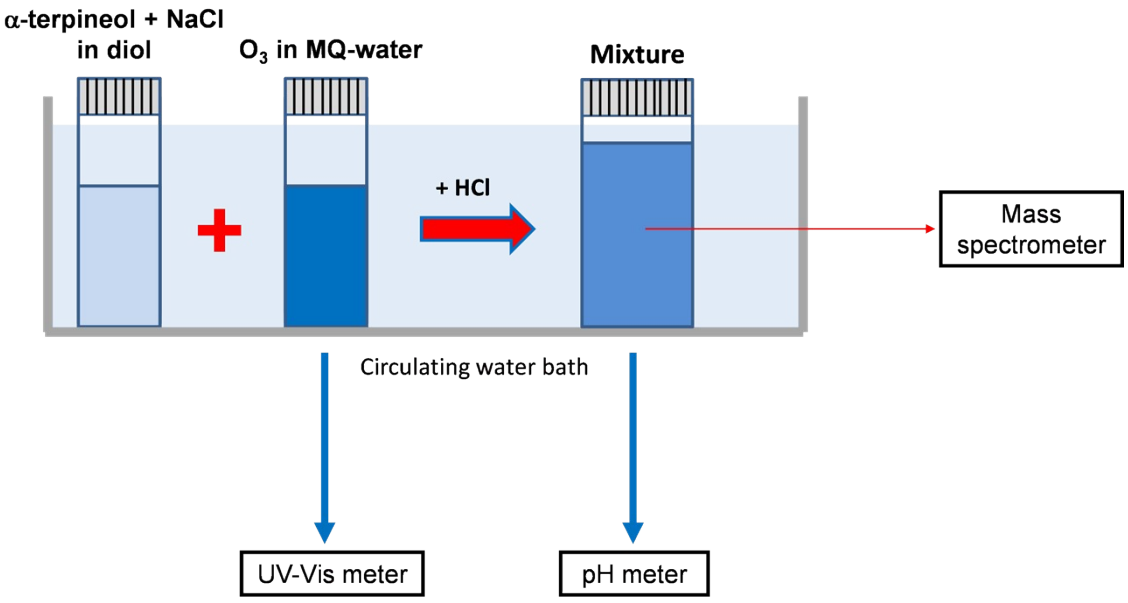

Figure S1 – Schematic setup of present experiment.

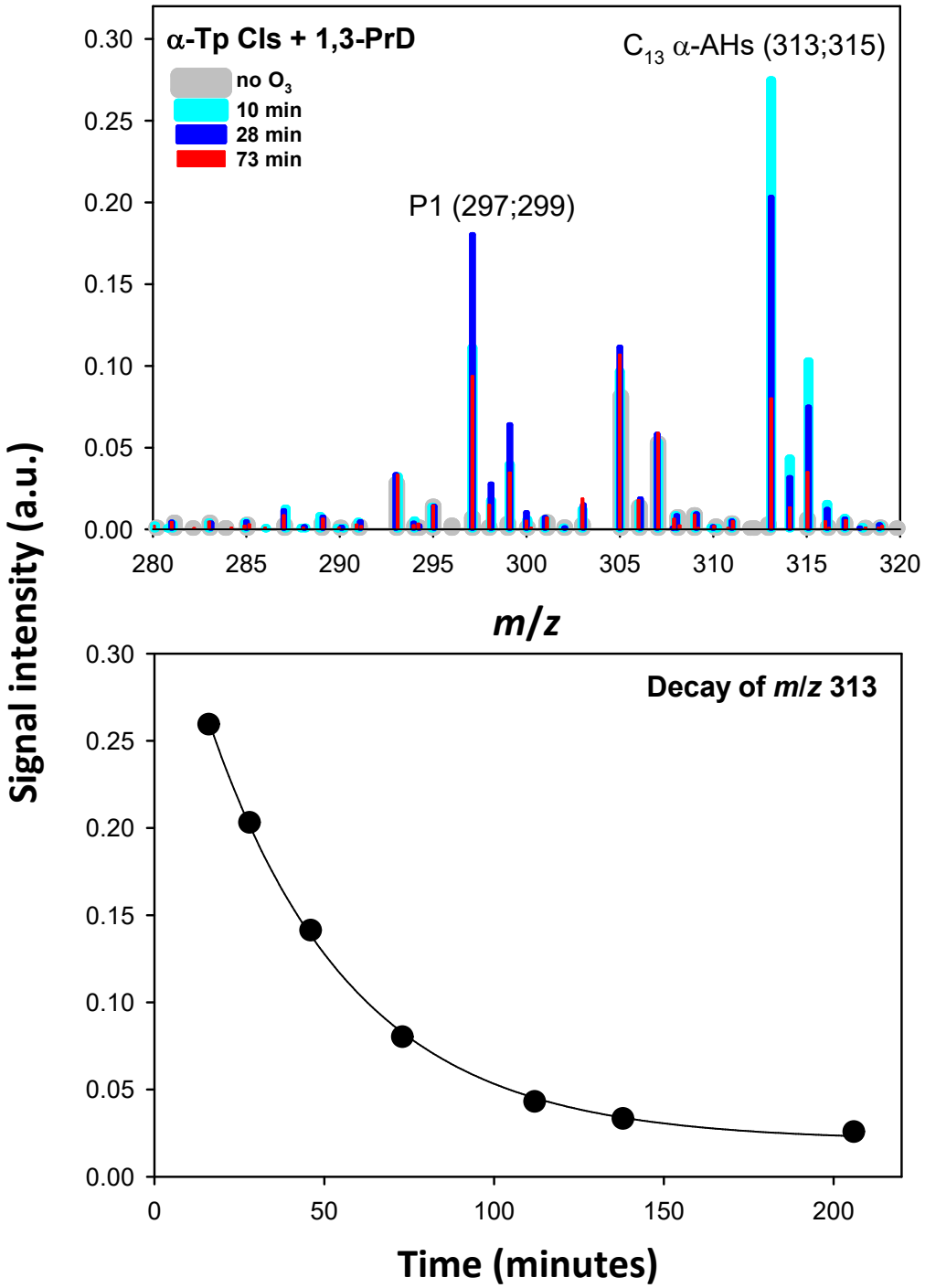

Fig. S2. Upper panel) Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of α-terpineol (1 mM)/NaCl (0.2 mM) in 1,3-propanediol:H_2O (1:1 = vol:vol) solution at pH 5.1 and *T* = 299 ± 1 K. Lower panel) The signal intensity at *m/z* 313 (C_{13} α-AHs) as a function of time.

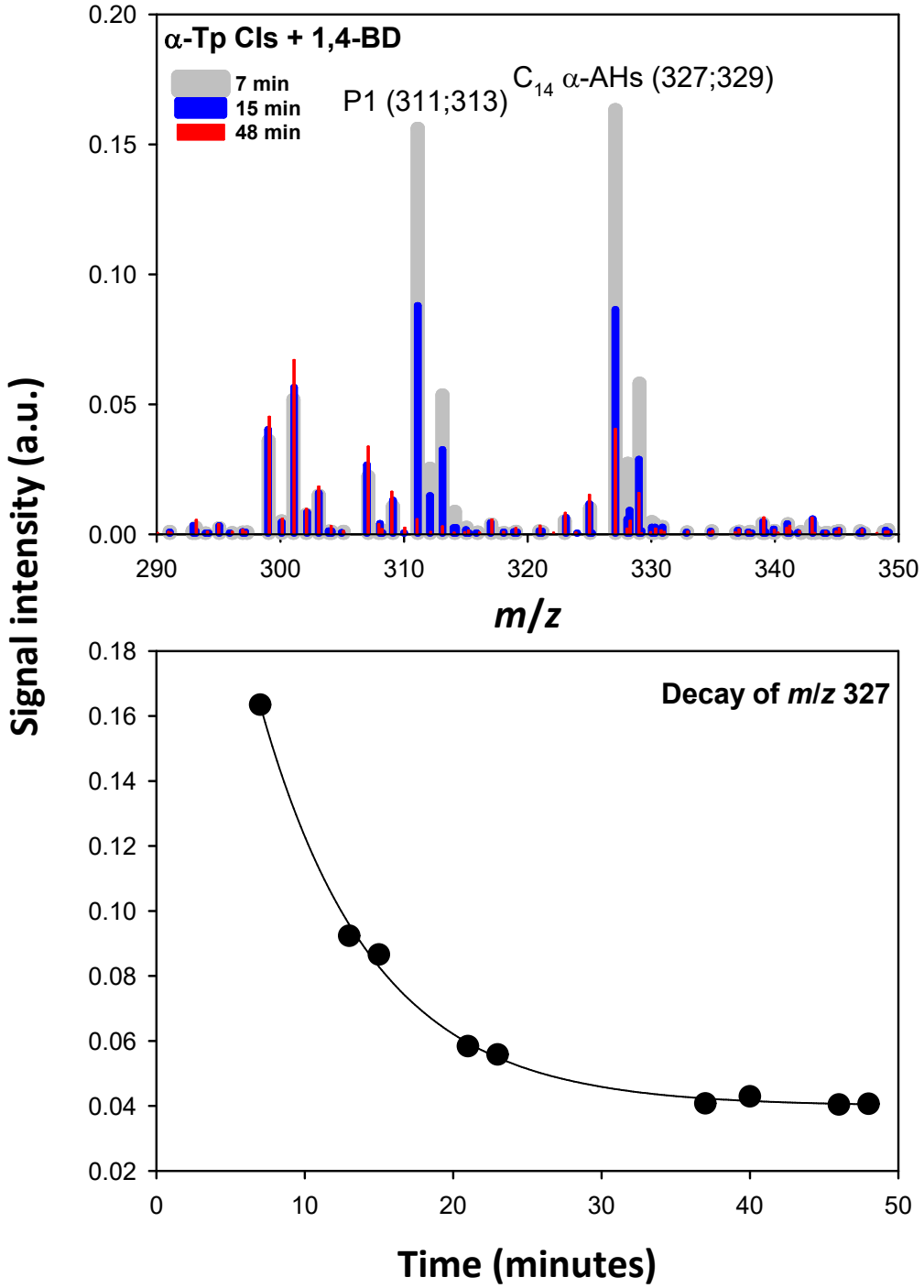

Fig. S3. Upper panel) Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of α-terpineol (1 mM)/NaCl (0.2 mM) in 1,4-butanediol:H_2O (1:1 = vol:vol) solution at pH 4.5 and T = 299 ± 1 K. Lower panel) The signal intensity at m/z 327 (C_{14} α-AHs) as a function of time.

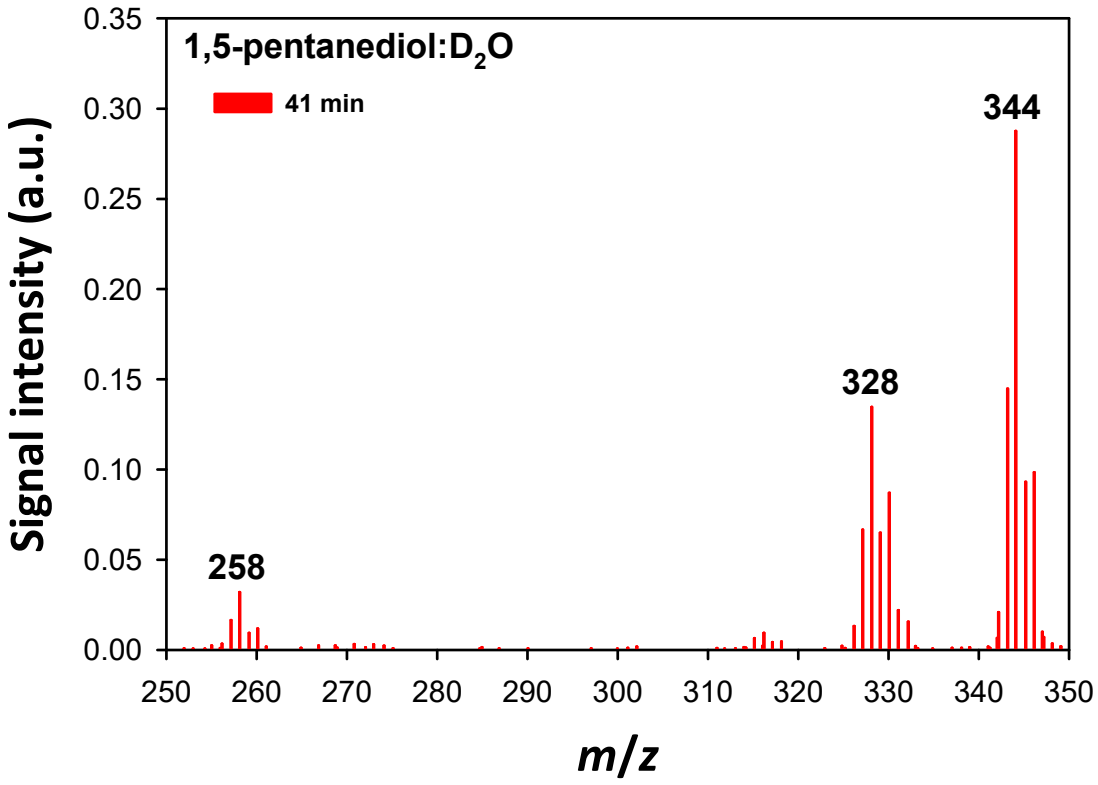

Fig. S4. Negative-ion mass spectra of mixtures obtained by ozonolysis ($[O_3]_0$ = 0.06 ± 0.01 mM) of α-terpineol (1 mM)/NaCl (0.2 mM)/HCl (0.05 mM) in 1,5-pentanediol:D_2O (1:1 = vol:vol) solution at pD = 5.8 at *T* = 299 ± 1 K.

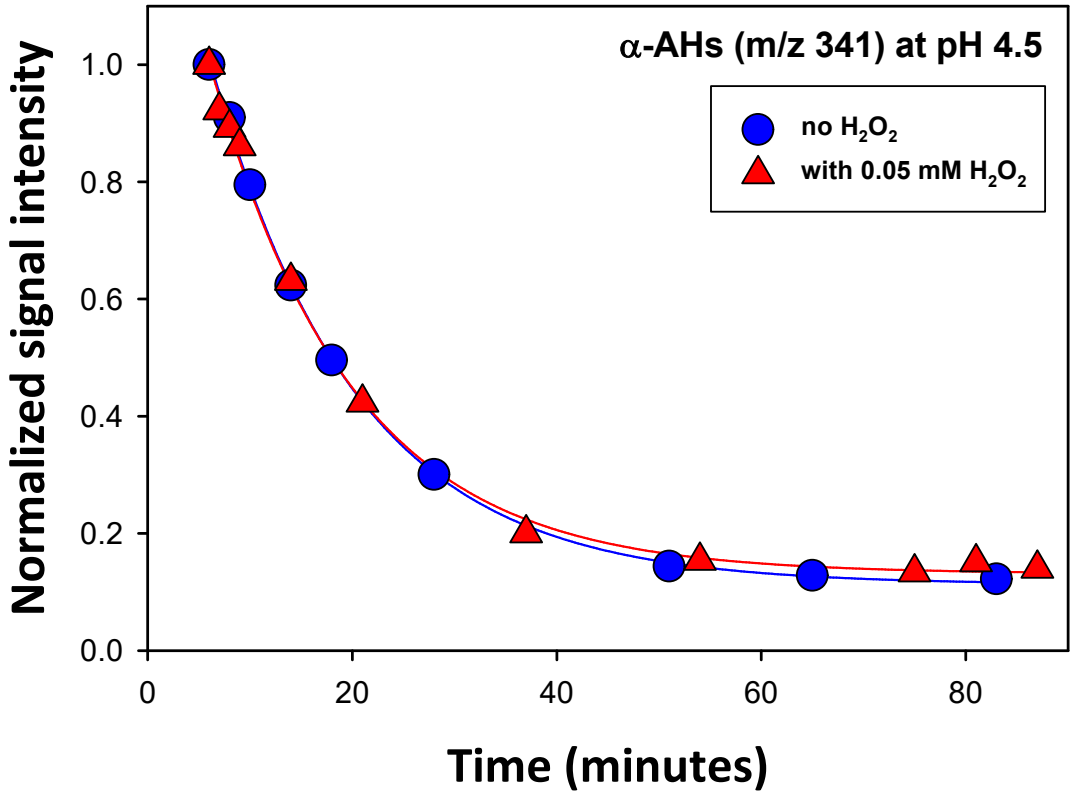

Fig. S5 Temporal profiles of the Cl^- adducts of the α-AHs (*m/z* 341) generated by ozonolysis of (1 mM α-terpineol and 0.2 mM NaCl) at $[O_3]_0$ = 0.06 ± 0.01 mM in a 1,5-pentanediol:water (1:1 = vol:vol) solution in the absence (blue circles) or presence of 0.05 mM H_2O_2 (red triangles) at T = 299 ± 1 K acidified by 0.05 mM to pH 4.5. Background signals obtained from mass spectra in the absence of O_3 were subtracted. Lines indicate fits of signal intensities (S) to single-exponential functions with baselines.

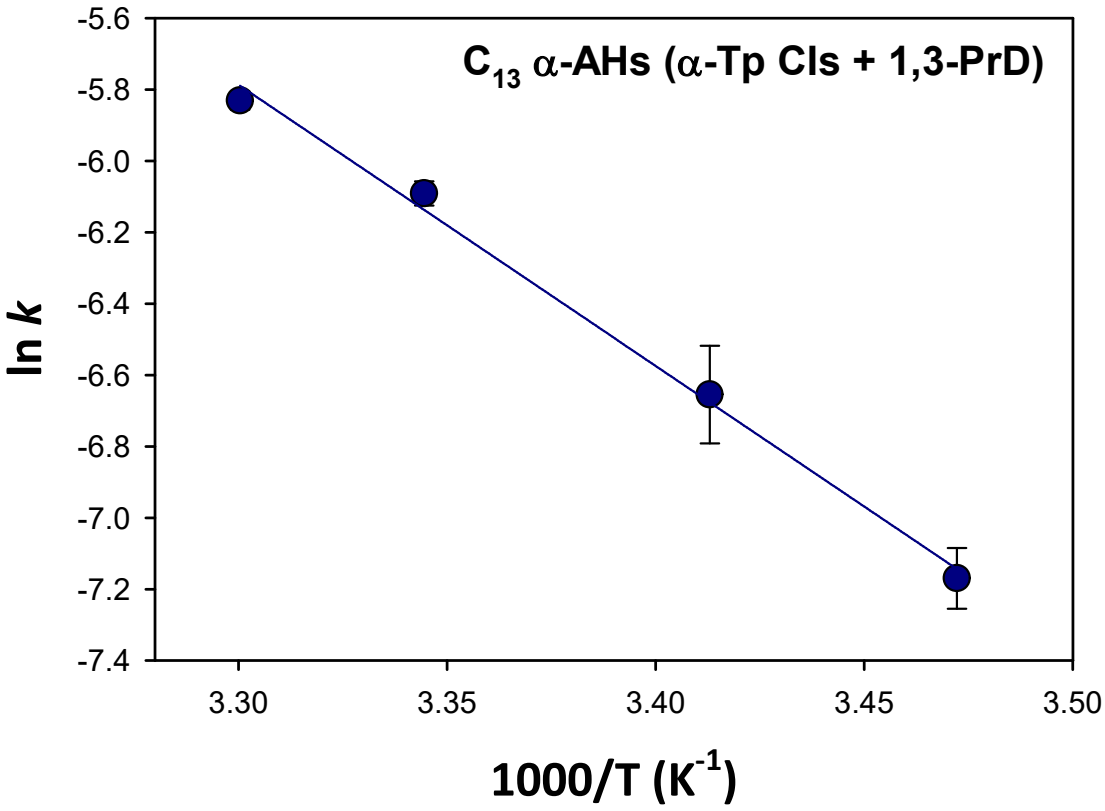

Fig. S6. Arrhenius plot of the rate coefficients for decay of the C_{13} α-AHs generated by ozonolysis of α-terpineol/NaCl in 1,3-propanediol:water (1:1) at pH 4.5. Note the error bars (= SDs) are obscured by the symbols in some cases. The linear regression yielded a preexponential factor (A) of 6.0×10^8 s^{-1} (ln A = 20.2 ± 1.3) and an E_a value of 15.7 ± 0.8 kcal mol^{-1}.

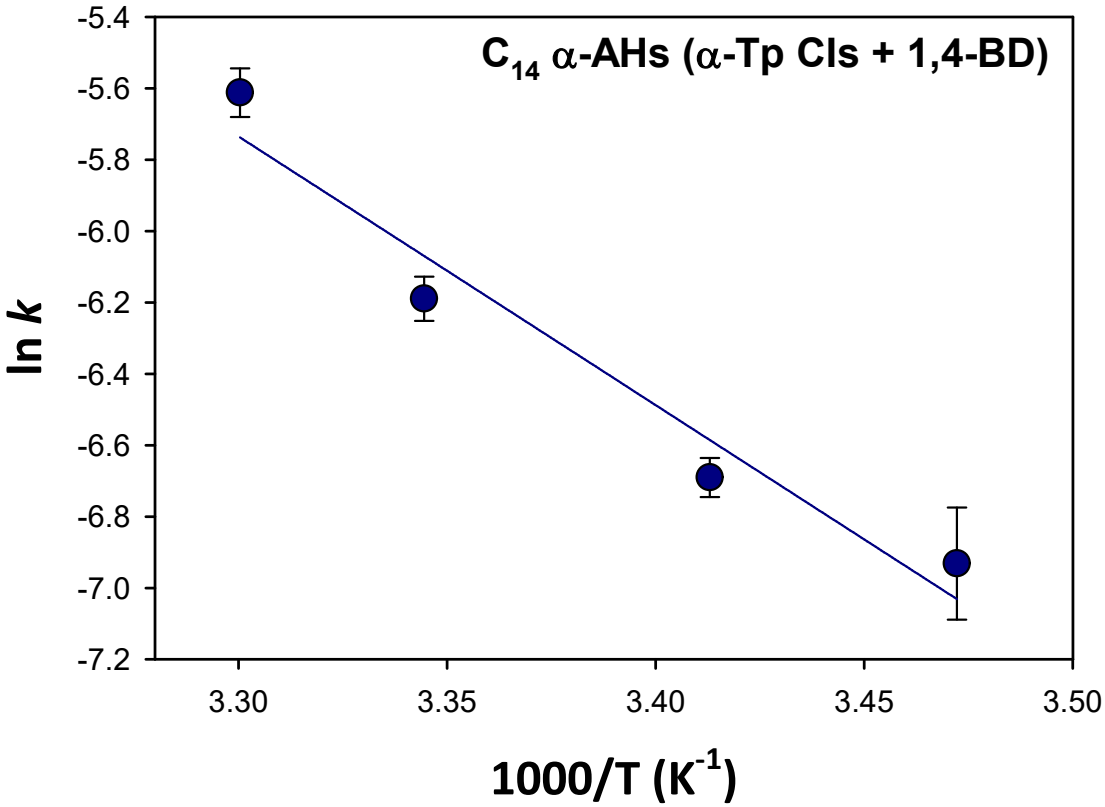

Fig. S7. Arrhenius plot of the rate coefficients for decay of the C_{14} α-AHs generated by ozonolysis of α-terpineol/NaCl in 1,4-butanediol:water (1:1) at pH 4.5. The linear regression yielded a preexponential factor (*A*) of 2.0×10^8 s^{-1} (ln *A* = 19.1 ± 4.1) and an E_a value of 15.0 ± 2.4 kcal mol^{-1}.