SUPPORTING INFORMATION

Identification and Quantification of 4-Nitrocatechol Formed from OH and NO_3 Radical-Initiated Reactions of Catechol in Air in the Presence of NO_x: Implications for Secondary Organic Aerosol Formation from Biomass Burning

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Contents: The supporting information contains the following information: HPLC calibration curves of 4NC and 5-nitro-1,2,3-benzenetriol; UV-Vis spectra of 4NC and 5-nitro-1,2,3-benzenetriol; proposed electron ionization mechanism for 4NC; thermal desorption profiles of SOA and 4NC; photograph of SOA collected on Teflon filters; HPLC chromatogram of SOA; CI-ITMS mass spectra of 5-nitro-1,2,3-benzenetriol; HPLC chromatogram of carbonyl derivatized SOA; and references.

Number of Pages: 8
Number of Figures: 10
Number of References: 2

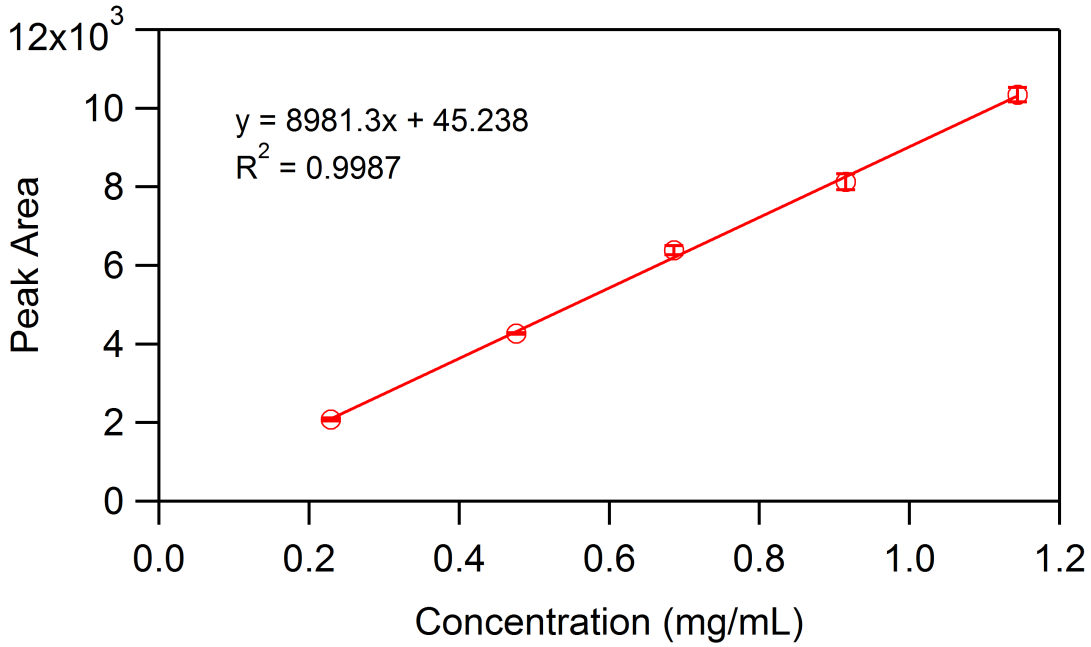

Figure S1. HPLC calibration curve of 4NC absorbance measured at λ = 360 nm.

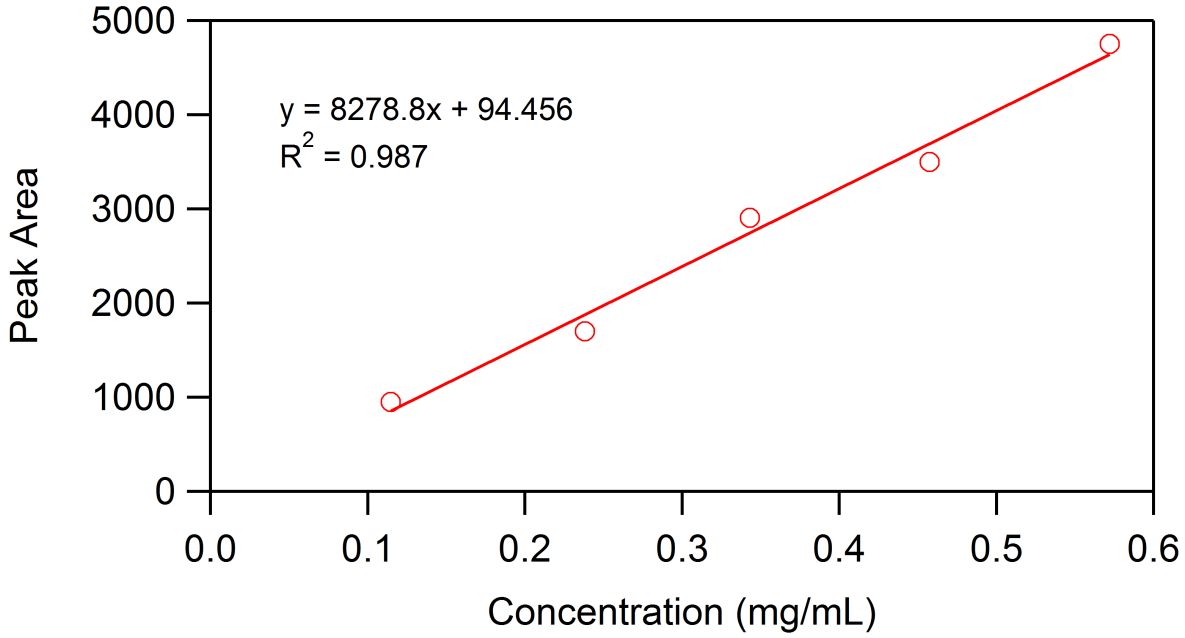

Figure S2. HPLC calibration curve of 5-nitro-1,2,3-benzenetriol measured at λ = 253 nm.

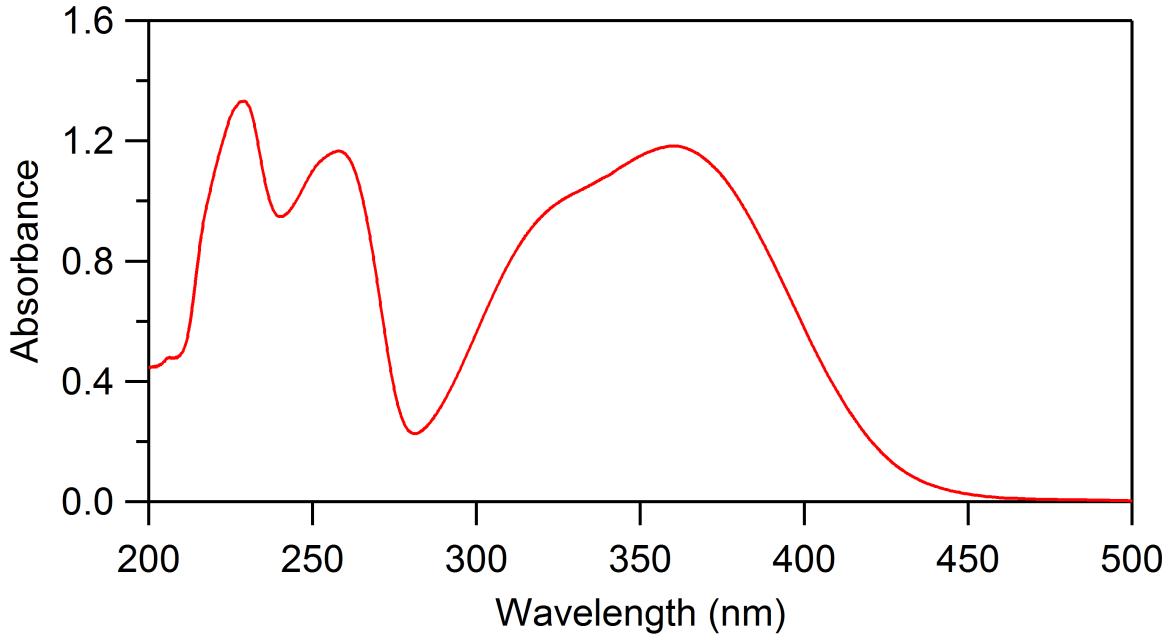

Figure S3. UV-Vis spectrum of 1.76 x 10^{-4} M 4NC in methanol measured with a spectrophotometer.

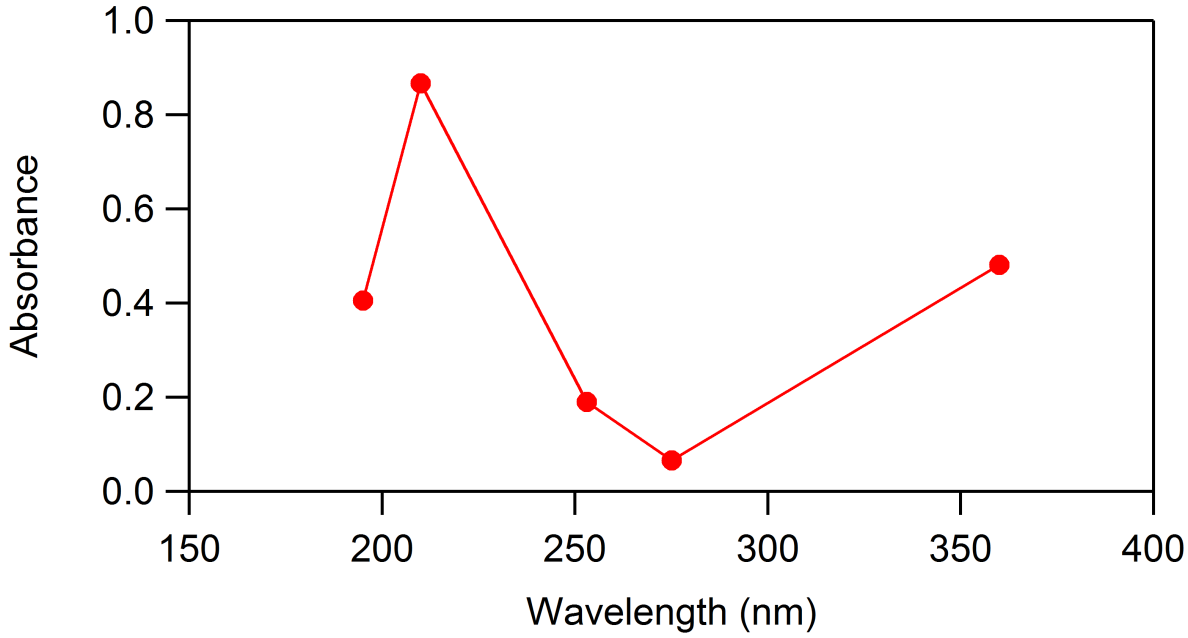

Figure S4. Reconstructed UV-Vis spectrum of 0.1145 mg/mL solution of 5-nitro-1,2,3-benzenetriol using peak areas from HPLC multiwavelength detection at 195 nm, 210 nm, 253 nm, 275 nm and 360 nm. The lines between points are linear interpolations, and are not indicative of structure between measured points. Absorbance values are relative.

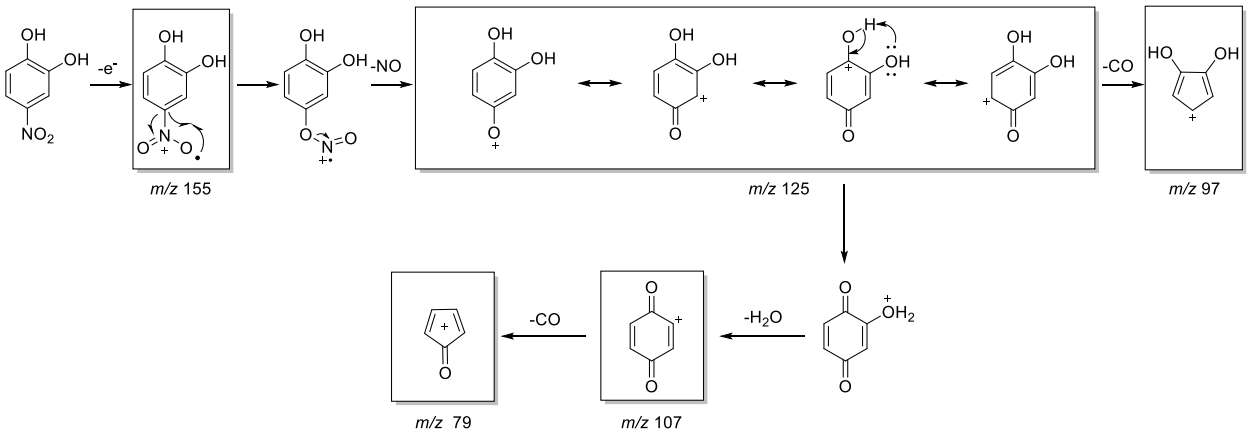

Figure S5. Proposed mechanism for formation of major ions observed in TDPBMS electron impact ionization mass spectrum of 4NC.

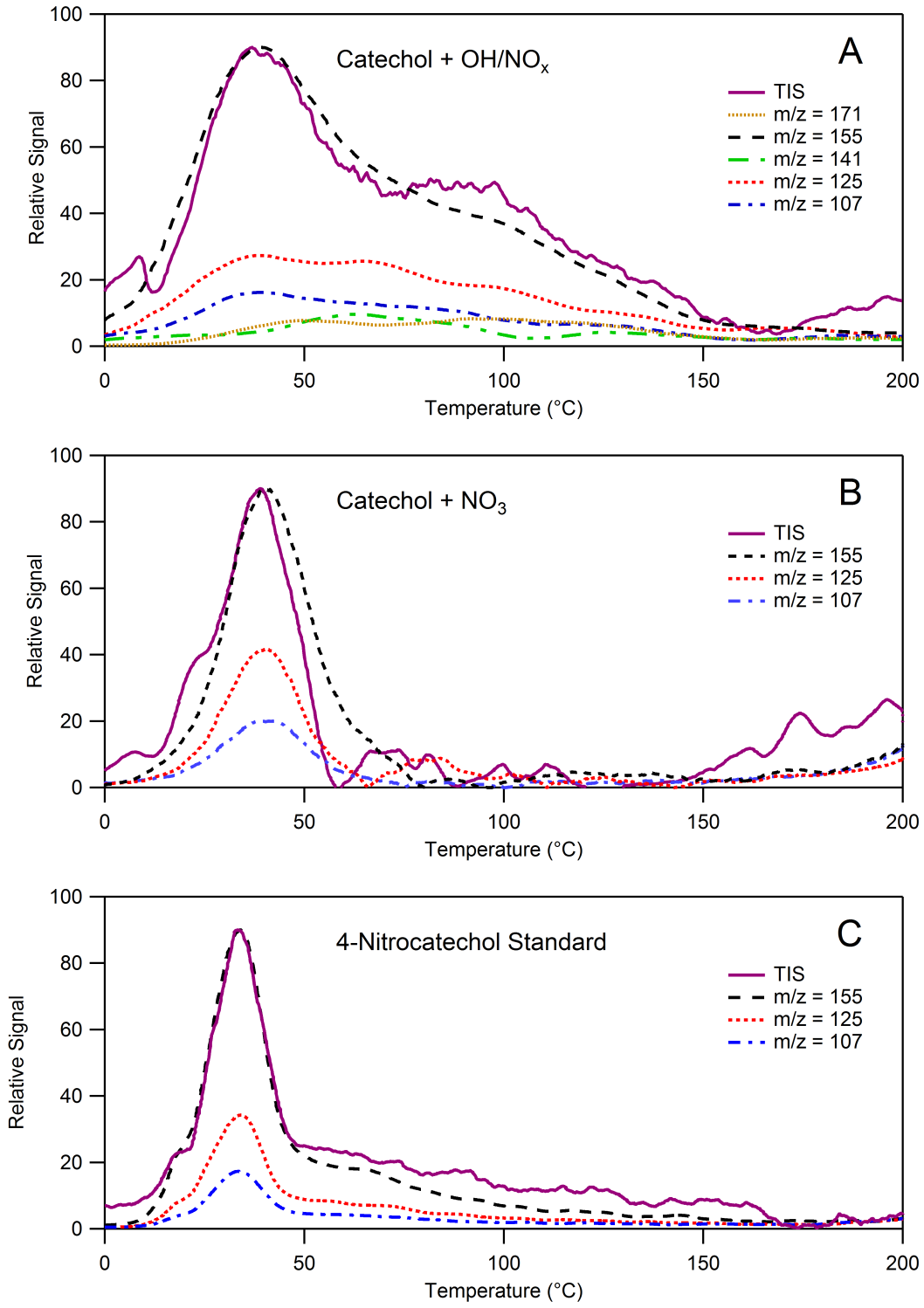

Figure S6. Thermal desorption profiles of total ion signal (TIS) and characteristic ions for SOA formed from reactions of catechol with (A) OH radicals and (B) NO_3 radicals, and (C) aerosol formed from atomization of a 4NC standard. The contribution of DOS seed particles to the TIS in (A) and (B) has been removed.

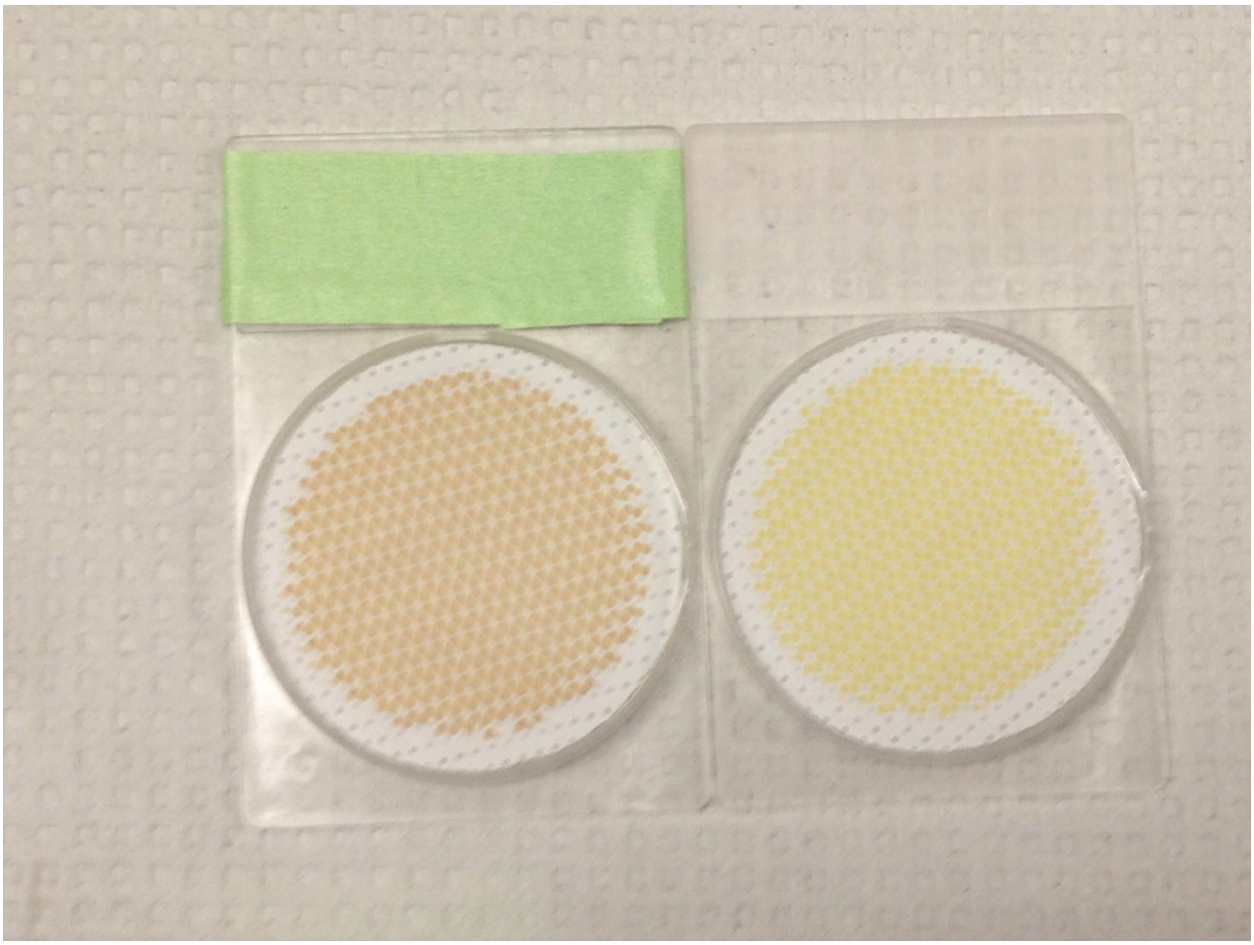

Figure S7. Secondary organic aerosol collected on Teflon filters for reactions of catechol with OH radicals (left) and NO_3 radicals (right).

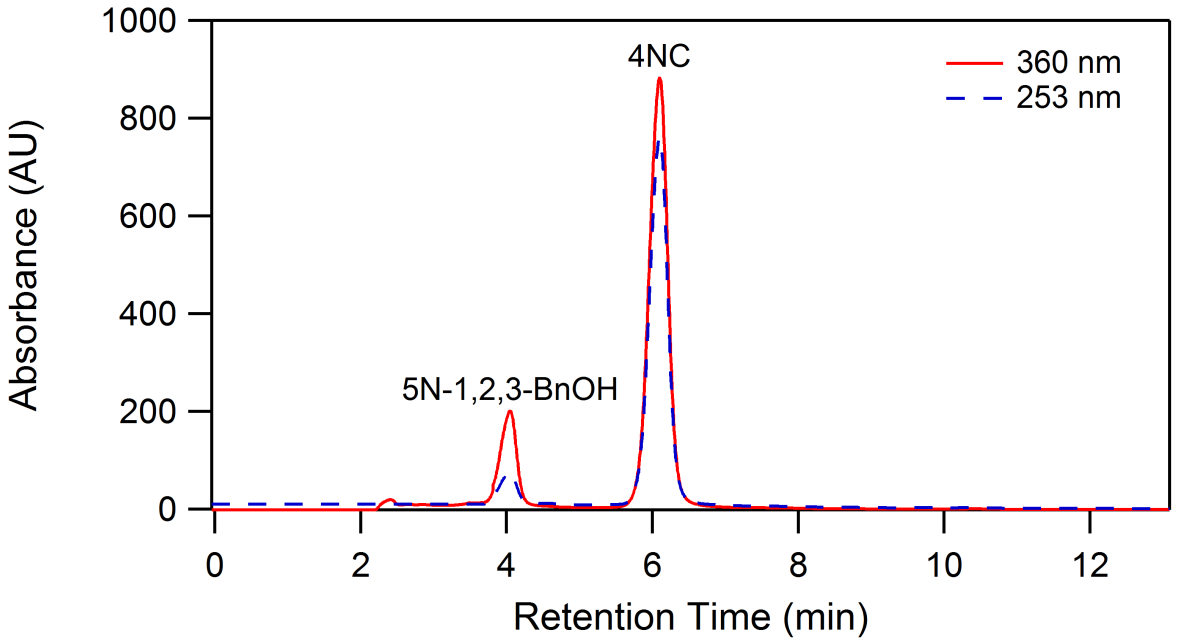

Figure S8. HPLC chromatogram of SOA formed from the reaction of catechol with OH radicals. 5N-1,2,3-BnOH corresponds to 5-nitro-1,2,3-benzenetriol.

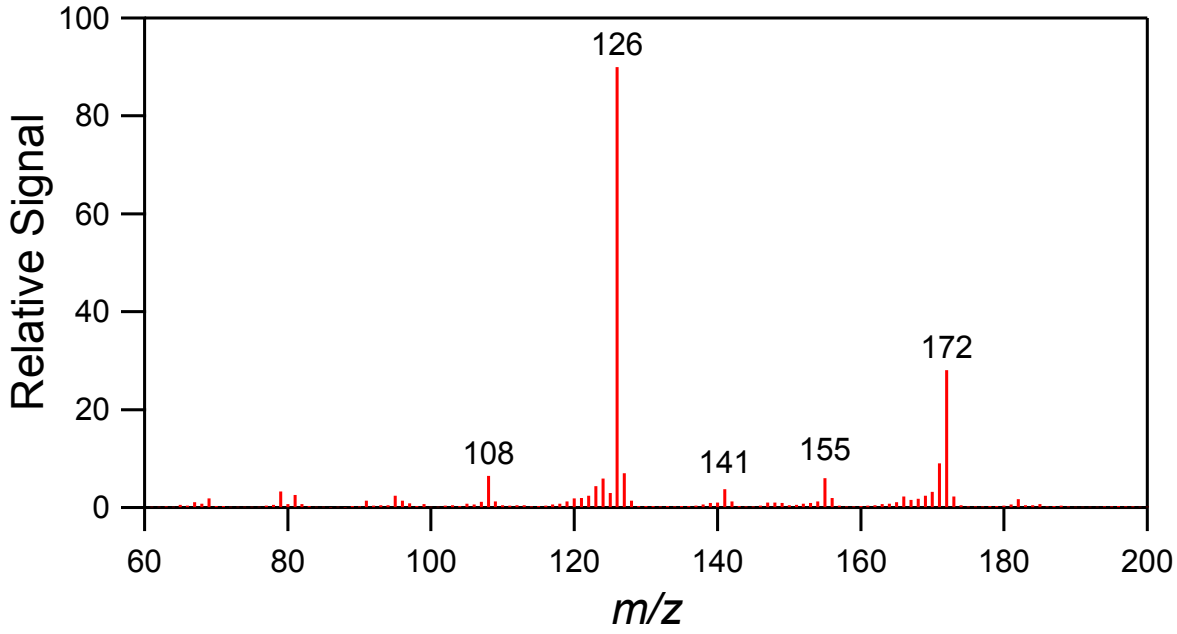

Figure S9. Mass spectrum of 5-nitro-1,2,3-benzenetriol obtained by HPLC fractionation and CI-ITMS analysis of SOA formed from the reaction of catechol with OH radicals.

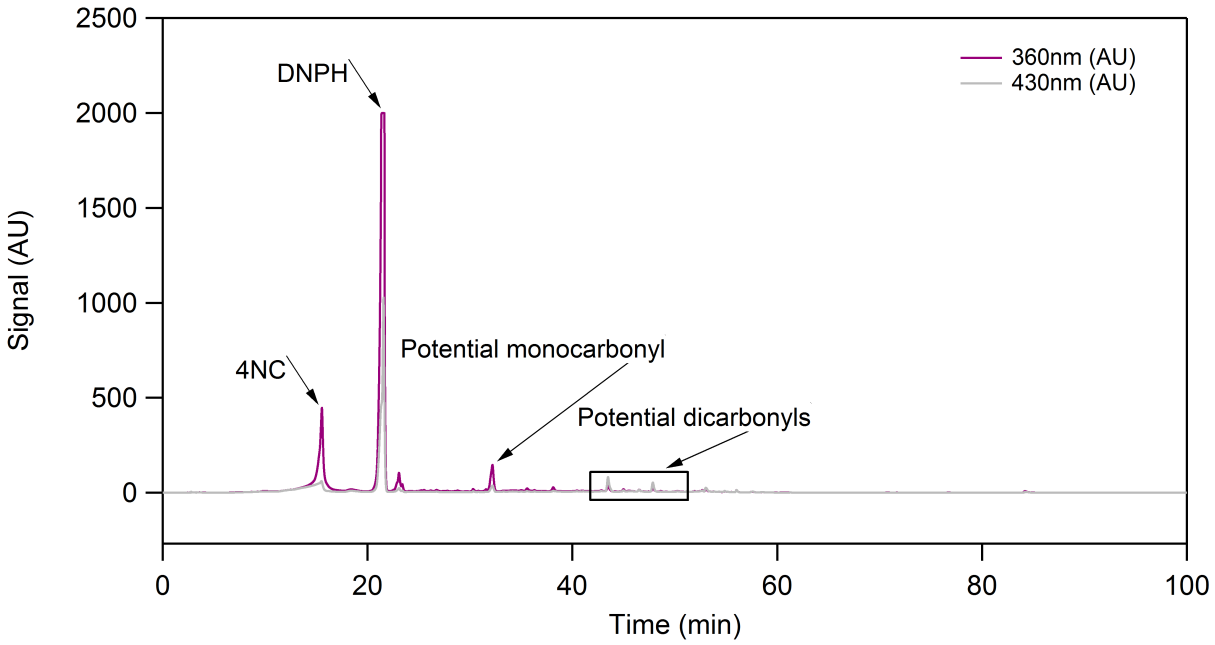

Figure S10. HPLC chromatogram from carbonyl derivatized SOA fromed from reaction of catechol with OH radicals. Retention time for 4NC differs from previous chromatogram due to use of mobile phase according to Ranney and Ziemann.[1] Monocarbonyl and dicarbonyl assignments are based on 2:1 ratio of absorbance at 360 nm relative to 430 nm as described by Grosjean et al.[2]

References

1. Ranney, A. P.; Ziemann, P. J. Identification and quantification of oxidized organic aerosol compounds using derivatization, liquid chromatography, and chemical ionization mass spectrometry. *Aerosol Sci. Technol.* **2017**, *51*, 342–353.

2. Grosjean, E.; Green, P. G.; Grosjean, D. Liquid chromatography analysis of carbonyl (2,4-dinitrophenyl)hydrazones with detection by diode array ultraviolet spectroscopy and by atmospheric pressure negative chemical ionization mass spectrometry. *Anal. Chem.* **1999**, *71*, 1851–1861.