Supporting information for

"Light Absorption of Secondary Organic Aerosol: Composition and Contribution of Nitro-aromatic Compounds"

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Table Number: 12

Figure Number: 14

Page number: 50

METHODS

1. UV-vis analysis

A 1.5 cm^2 punch of each filter sample was extracted with 5 mL methanol (HPLC grade, Thermo Fisher Scientific) ultrasonically for 15 min, followed by filtration through a 0.2 μm pore size polytetrafluoroethylene (PTFE) filter head using a glass syringe. The light absorption (A_λ) of filtered extracts was measured with a UV-vis spectrometer at λ = 200-900 nm and resolution of 0.2 nm (V660, Jasco Inc., Easton, MD). This work focused on the light absorption at λ = 300-550 nm, where most of the BrC absorption has been observed.[1] A reference cuvette containing methanol was used to eliminate the solvent effect on absorption. In addition, the light absorption of blank filter extract (close to 0) was used for correction. The wavelength accuracy and repeatability were monitored on a monthly basis to ensure the quality of collected data. The wavelength accuracy is less than ± 0.3 nm and the wavelength repeatability is less than ± 0.05 nm. Many studies have shown that methanol can extract organic aerosol at very high efficiencies (> 90%), and a large fraction of light absorption in the near-UV and visible range is ascribed to water insoluble organic materials.[1-3] As such, we assumed that the secondary organic aerosol (SOA) in each filter sample was totally dissolved in the methanol extract, of which the light absorption reflected the total light absorption of each sample.

2. Calculation of imaginary refractive index

The optical properties of organic aerosol (OA) is commonly parameterized as complex refractive index ($m = n - ik$) in climate models.[4,5] The real (n) and the imaginary (k) parts of the refractive index reflect the scattering and absorbing properties, respectively. The imaginary part of the refractive index (k) of SOA generated from the chamber experiments were calculated from their spectroscopic data using eq. S1:[6,7]

$$k = \frac{\rho \times \lambda \times \mathrm{Abs}_\lambda}{4 \times \pi \times \mathrm{OM}} = \frac{\rho \times \lambda \times \mathrm{MAE}_\lambda}{4 \times \pi} \qquad \text{(S1)}$$

where Abs_λ (Mm^{-1}) is the light absorption coefficient, MAE_λ ($\mathrm{m}^2\ \mathrm{g}^{-1}$) is the bulk mass absorption efficiency, and OM ($\mu\mathrm{g\ m}^{-3}$) is the concentration of SOA and ρ ($\mathrm{g\ cm}^{-3}$) is the density of SOA. In this work, the density of SOA is assigned as 1.2 $\mathrm{g\ cm}^{-3}$ based on the estimate from Turpin and Lim[8] for organic aerosols.

3. HPLC/DAD-Q-ToFMS method

Target compounds separation was fulfilled using a Zorbax Eclipse Plus C18 column (2.1×100 mm, 1.8 μm particle size, Agilent Technologies) with an injection volume of 2 μL and flow rate of 0.2 mL/min. The column temperature was kept at 40 °C, and the gradient separation was conducted with 0.2% acetic acid (v/v) in water (eluent A) and methanol (eluent B). The concentration of eluent B was 25% for the first 3 min, increased to 100% from 3 to 10 min, held at 100% from 10 to 32 min, and then decreased back to 25% from 32 to 37 min. The DAD monitored absorbance of each sample from 200 to 900 nm with a step of 2 nm. For ease of analysis, we focused on the signal at 365 ± 10 nm, which is a general measure of chromophore components in sample extracts.

The Agilent 6520 series Accurate Mass Q-ToFMS instrument was equipped with a multimode ion source operated under the electrospray ionization (ESI) negative (-) ion mode. The ion source conditions used a 2000 V capillary voltage, 140 V fragmentor voltage, 65 V skimmer voltage, 300 °C gas temperature, 5 $\mathrm{L\ min}^{-1}$ drying gas flow rate and 40 psig nebulizer. The ESI-Q-ToFMS instrument acquired mass spectra from m/z 40 to 1000 at rate of 3 spectra s^{-1}. At the beginning of each batch analysis, the Q-ToFMS instrument was calibrated by a diluted commercial available tuning mixture (Agilent G1969-85020). The specific ions included in the tuning mixture were 112.985587, 301.998139, 601.978977, 1033.988109, 1333.968947,

1633.949786, 1933.930624 and 2233.911463. During the running of each sample, the Q-ToFMS was continuously tuned through the injection of purine and HP-0921 acetate adduct (Agilent G1969-85001). The Mass Hunter Version B.05.01 Build 5.01.5125.3 software was used to acquire the data.

4. MAE_λ calculation for standard compounds

Methanol solution of standard compounds were diluted in series and analyzed by UV-vis spectrometer (scan from 200 to 900 nm). The UV-vis spectra of standard compounds at around 1 ng μL^{-1} are shown in Figure S11. The 3,5-dinitrocatechol, a surrogate standard representing the light-absorbing characteristics of $C_6H_4N_2O_6$ in the identified compounds, could not be detected with HPLC/DAD-Q-ToFMS using the method in this work, which might be associated with its poor ionization efficiency. As such, it was not used for the quantification of $C_6H_4N_2O_6$.

The MAE_λ ($m^2\ g^{-1}$) for each standard compound could be calculated as:

$$MAE_\lambda = \frac{Abs_\lambda^*}{C_l} \qquad (S2)$$

where Abs_λ^* (m^{-1}) is the light absorption coefficient of each standard compound in methanol solution; C_l (ng μL^{-1}) is the concentration of each standard compound in methanol solution.

The Abs_λ^* could be obtained from the following equation.

$$Abs_\lambda^* = \frac{(A_\lambda - A_{700}) \times \ln(10)}{L} \qquad (S3)$$

Here, A_λ and A_{700} come from the UV-vis spectrometer; L is the optical path length of the quartz cuvette (0.01 m) in the UV-vis spectrometer.

Combining eqs. S2 and S3, $A_\lambda - A_{700}$ and C_l are linearly related as:

$$A_\lambda - A_{700} = MAE_\lambda \times C_l \times \frac{L}{\ln(10)} \qquad (S4)$$

For most of the standard compounds, the Beer-Lambert law is valid in the whole concentration range, and the MAE_λ could be obtained from the slope of the linear regression between $A_\lambda - A_{700}$ and C_l.

However, the Beer-Lambert law is not valid for some standard compounds at high concentrations. Interestingly, $A_\lambda - A_{700}$ is still linearly related to C_l, but the intercept value is not 0. Then eq. S4 could be rewritten as:

$$A_\lambda - A_{700} = MAE_\lambda' \times C_l \times \frac{L}{\ln(10)} + b \times \frac{L}{\ln(10)} \qquad (S5)$$

where $b \times L/\ln(10)$ (m^{-1}) is the intercept; the slope of the linear regression between $A_\lambda - A_{700}$ and C_l was assumed to be directly related to MAE_λ'. The MAE_λ values of standard compounds at different concentration ranges and wavelengths were provided in Table S4.

5. Abs_λ attribution for identified compounds

To estimate the contribution of each identified nitro-aromatic compound to the total light absorption of each SOA sample, the Abs_λ (Mm^{-1}) of each identified compound was calculated using eq.1 of the manuscript.

$$Abs_\lambda = (A_\lambda - A_{700}) \times \frac{V_l}{V_a \times L} \ln(10) \qquad (1)$$

where V_l (m^3) is the volume of methanol (5 mL) used for extraction and V_a (m^3) is the volume of the sampled air.

In the concentration range where the Beer-Lambert law is valid, the Abs_λ of each identified compound could be obtained by combining eqs. S4 and 1.

$$Abs_\lambda = MAE_\lambda \times C_l \times \frac{L}{\ln(10)} \times \frac{V_l}{V_a \times L} \ln(10) = MAE_\lambda \times C_a \qquad (S6)$$

where C_a ($ng\ m^{-3}$) is the concentration of identified compounds in the air.

While in the high concentration range of some compounds where the Beer-Lambert law is not valid, the Abs_λ of each identified compound could be obtained by combining eqs. S5 and 1.

$$\mathrm{Abs}_\lambda = (\mathrm{MAE}_\lambda' \times C_l \times \frac{L}{\ln(10)} + b \times \frac{L}{\ln(10)}) \times \frac{V_l}{V_a \times L} \ln(10) = \mathrm{MAE}_\lambda' \times C_a + b \times \frac{V_l}{V_a} \quad \text{(S7)}$$

For simplicity, only 5 representative wavelength (365, 400, 450, 500, 550 nm) in the range of 300 – 550 nm were selected for Abs_λ attribution. The method used for Abs_λ attribution in this work presumes that the light absorption of each identified compound in sample extracts is not impacted by other components, which needs to be evaluated in further study.

Table S1. Summary of experimental conditions and sample information in this work.

Experiment ID	Filter ID	VOC type	Oxidant	Humidity (%)	Initial [NO_X] ppm	Initial [H_2O_2] ppm	Initial [VOC] ppmC	ΔVOC[a] ppmC	SOA yield	V (m^3)[b]	SOA Conc.[c] (μg m^{-3})
ER605	GF2	α-Pinene	NO_X	18.5	0.25	/	1.61	1.35	0.056	26.5	31.6
ER618	GF4	α-Pinene	NO_X	10.1	0.30	/	2.88	2.78	0.095	18.4	103
ER636	GF2	α-Pinene	NO_X	18.4	0.20	/	1.43	1.21	0.046	29.7	22.4
ER726	GF2	α-Pinene	NO_X	10.5	0.074	/	1.10	0.98	0.065	22.4	24.4
ER606	GF2	α-Pinene	H_2O_2	18.7	/	6.23	1.01	0.88	0.25	26.8	94.8
ER620	GF4	α-Pinene	H_2O_2	10.1	/	2.55	1.05	1.02	0.20	18.4	77.1
ER633	GF2	Isoprene	NO_X	18.5	0.35	/	5.81	5.45	0.007	29.6	15.2
ER728	GF2	Isoprene	NO_X	10.3	0.49	/	6.68	6.19	0.005	19.6	11.0
ER729	GF2	Isoprene	NO_X	10.2	0.79	/	8.52	8.25	0.007	16.8	18.7
ER629	GF2	Isoprene	H_2O_2	18.6	/	4.79	5.45	3.67	0.025	29.6	38.5
ER630	GF2	Isoprene	H_2O_2	18.6	/	13.6	2.17	1.84	0.040	33.3	31.1
ER393	GF2	β-Caryophyllene	NO_X	10.2	0.21	/	0.45	0.35	0.42	21.4	57.1
ER716	GF2	β-Caryophyllene	NO_X	9.82	0.099	/	0.73	N.A.[d]	N.A.[d]	16.8	123
ER533	GF3	β-Caryophyllene	H_2O_2	10.2	/	0.26	0.39	0.39	0.51	20.5	81.4
ER693	GF2	β-Caryophyllene	H_2O_2	20.7	/	12.7	0.51	0.49	0.86	23.4	180
ER538	GF2	1,3,5-Trimethylbenzene	NO_X	15.8	0.50	/	4.51	3.97	0.016	19.0	25.8
ER752	GF5	1,3,5-Trimethylbenzene	NO_X	13.1	0.36	/	7.56	2.80	0.074	17.1	82.2
ER536	GF2	1,3,5-Trimethylbenzene	H_2O_2	16.0	/	3.53	6.41	4.91	0.063	18.1	128
ER536	GF5	1,3,5-Trimethylbenzene	H_2O_2	16.0	/	1.76	6.54	4.43	0.031	18.3	57.3
ER388	GF5	1,2,4-Trimethylbenzene	NO_X	10.3	0.25	/	12.56	7.76	0.020	39.4	54.5
ER753	GF5	1,2,4-Trimethylbenzene	NO_X	12.1	0.39	/	7.13	3.20	0.047	17.1	58.5
ER435	GF2	1,2,4-Trimethylbenzene	H_2O_2	10.2	/	3.49	6.09	3.74	0.084	18.9	117
ER435	GF5	1,2,4-Trimethylbenzene	H_2O_2	10.2	/	6.98	6.21	4.89	0.12	18.6	215
ER435	GF8	1,2,4-Trimethylbenzene	H_2O_2	10.2	/	1.74	6.26	3.14	0.050	18.9	58.3

[a] Reacted VOC concentration; [b] filter sample volume; [c] concentrations of SOA based on filter weight change and sample volume; [d] not available; [e] CH_3ONO was added and the concentration ranged from 0.072 to 0.083 ppmC.

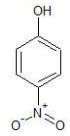
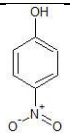
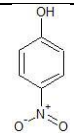
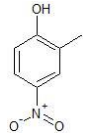
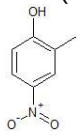
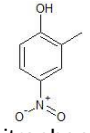
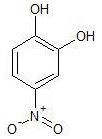
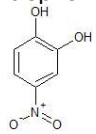
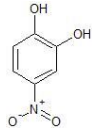
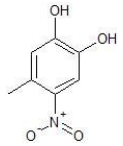
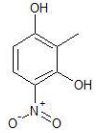
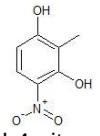
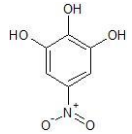
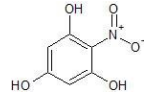
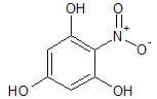
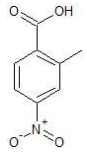
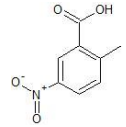
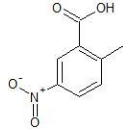
Table S1. Continue

Experiment ID	Filter ID	VOC	Oxidant	Humidity (%)	Initial [NO_X] ppm	Initial [H_2O_2] ppm	Initial [VOC] ppmC	ΔVOC[a] ppmC	SOA yield	V (m^3)[b]	SOA Conc.[c] (μg m^{-3})
ER366	GF2	m-Xylene	NO_X	10.5	0.42	/	12.3	6.96	0.051	17.3	130
ER610	GF2	m-Xylene	NO_X	19.0	0.27	/	5.27	3.28	0.058	26.9	69.9
ER695	GF2	m-Xylene	NO_X	20.7	0.34	/	7.45	5.21	0.045	23.5	97.3
ER751	GF5	m-Xylene	NO_X	12.2	0.29	/	5.53	3.23	0.059	17.1	74.7
ER429	GF6	m-Xylene	H_2O_2	14.6	/	5.85	5.39	2.65	0.11	27.3	112
ER430	GF2	m-Xylene	H_2O_2	10.2	/	4.41	4.86	2.45	0.14	20.7	118
ER430	GF6	m-Xylene	H_2O_2	10.2	/	4.41	5.08	2.15	0.077	18.9	59.9
ER612	GF2	m-Xylene	H_2O_2	18.7	/	2.46	2.10	1.31	0.052	26.9	29.2
ER613	GF2	m-Xylene	H_2O_2	18.7	/	2.54	2.75	1.36	0.075	26.9	42.1
ER634	GF2	Toluene	NO_X	18.9	0.32	/	7.11	2.82	0.094	29.7	109
ER634	GF4	Toluene	NO_X	18.9	0.32	/	4.98	1.86	0.051	29.7	39.2
ER694	GF2	Toluene	NO_X	19.1	0.35	/	5.50	2.64	0.051	23.5	56.1
ER700	GF2	Toluene	NO_X	7.64	0.32	/	4.42	2.61	0.082	14.2	71.5
ER701	GF2	Toluene	NO_X	9.73	0.30	/	4.55	2.41	0.078	16.7	72.8
ER702	GF2	Toluene	NO_X	8.09	0.31	/	4.29	2.90	0.090	12.3	71.1
ER744	GF2	Toluene	NO_X	11.3	0.30	/	5.05	2.34	0.067	17.0	58.9
ER745	GF2	Toluene	NO_X	9.44	0.19	/	5.13	3.19	0.079	12.1	70.3
ER755	GF5	Toluene	NO_X	12.3	0.30	/	6.05	2.53	0.12	17.1	117
ER433	GF2	Toluene	H_2O_2	10.2	/	6.17	5.46	2.29	0.20	18.9	170
ER541	GF2	Toluene	H_2O_2	15.8	/	3.10	2.18	0.97	0.085	30.3	33.4
ER553	GF2	Toluene	H_2O_2	16.0	/	11.1	2.90	1.41	0.078	21.3	42.8
ER772	GF5	Toluene	H_2O_2	11.7	/	7.92	6.09	1.70	0.16	18.3	101
ER390	GF3	Ethylbenzene	NO_X	10.2	0.22	/	11.0	3.76	0.056	21.4	78.3
ER754	GF8	Ethylbenzene	NO_X	12.3	0.27	/	6.37	1.99	0.13	17.1	98.5
ER759	GF2	Ethylbenzene	NO_X	19.1	0.23	/	4.08	0.82	0.075	17.1	26.1
ER760	GF2	Ethylbenzene	NO_X	11.4	0.19	/	3.79	1.79	0.11	8.60	58.3
ER761	GF2	Ethylbenzene	NO_X	11.6	0.19	/	3.63	1.46	0.077	14.9	37.9
ER762	GF2	Ethylbenzene	NO_X	11.8	0.20	/	3.62	1.09	0.062	17.1	25.3
ER770	GF2	Ethylbenzene	H_2O_2	12.1	/	7.20	4.51	1.29	0.065	17.5	32.3
ER770	GF5	Ethylbenzene	H_2O_2	12.1	/	7.20	4.52	1.26	0.047	17.5	22.7
ER770	GF8	Ethylbenzene	H_2O_2	12.1	/	7.20	4.53	1.35	0.096	17.5	51.9
ER770	GF11	Ethylbenzene	H_2O_2	12.1	/	7.20	4.53	1.38	0.077	17.6	41.4
ER773	GF5	Ethylbenzene	H_2O_2	11.9	/	7.83	4.72	1.67	0.14	17.5	87.5

Table S1. Continue

Experiment ID	Filter ID	VOC type	Oxidant	Humidity (%)	Initial [NO_X] ppm	Initial [H_2O_2] ppm	Initial [VOC] ppmC	ΔVOC[a] ppmC	SOA yield	V (m^3)[b]	SOA Conc.[c] (μg m^{-3})
ER542	GF2	Benzene[e]	NO_X	15.5	0.27	/	9.00	1.55	0.12	20.0	74.1
ER542	GF4	Benzene[e]	NO_X	15.5	0.27	/	9.41	1.92	0.061	30.2	47.2
ER543	GF2	Benzene[e]	NO_X	15.5	0.27	/	7.00	1.23	0.041	36.3	20.8
ER615	GF2	Benzene[e]	NO_X	18.5	0.25	/	7.44	0.97	0.064	26.8	25.2
ER704	GF2	Benzene	NO_X	25.5	0.18	/	8.11	1.36	0.087	28.2	47.0
ER705	GF2	Benzene	NO_X	9.94	0.29	/	8.10	1.34	0.055	19.7	27.4
ER756	GF5	Benzene	NO_X	12.2	0.28	/	12.7	2.82	0.36	17.1	383
ER763	GF4	Benzene	NO_X	12.0	0.18	/	12.7	2.21	0.16	17.1	136
ER544	GF2	Benzene	H_2O_2	15.5	/	2.89	3.97	0.94	0.075	35.1	28.2
ER614	GF2	Benzene	H_2O_2	18.5	/	4.44	4.67	0.73	0.055	26.9	16.6
ER706	GF2	Benzene	H_2O_2	10.3	/	9.43	9.34	2.78	0.064	20.2	66.7
ER771	GF2	Benzene	H_2O_2	11.7	/	6.98	8.01	1.61	0.063	18.2	26.7
ER771	GF5	Benzene	H_2O_2	11.7	/	6.98	8.00	1.54	0.046	17.4	24.2
ER703	GF2	Napthalene	NO_X	19.3	0.25	/	0.75	0.49	0.11	23.3	20.8
ER730	GF3	Napthalene	NO_X	10.3	0.28	/	0.67	0.35	0.29	22.4	38.3
ER767	GF5	Napthalene	NO_X	11.8	0.21	/	1.31	0.46	0.41	17.1	70.5
ER460	GF5	Napthalene	H_2O_2	15.3	/	2.12	0.81	0.66	0.38	20.3	106
ER774	GF2	Napthalene	H_2O_2	11.8	/	8.05	1.57	1.16	0.39	17.2	173
ER774	GF5	Napthalene	H_2O_2	11.8	/	8.05	1.57	1.18	0.37	17.2	164
ER707	GF3	m-Cresol	NO_X	10.2	0.27	/	1.65	1.22	0.18	17.2	83.7
ER713	GF3	m-Cresol	NO_X	10.4	0.11	/	2.97	1.44	0.73	16.2	479
ER749	GF5	m-Cresol	NO_X	12.6	0.087	/	0.71	0.66	0.29	17.1	85.8
ER776	GF2	m-Cresol	H_2O_2	11.6	/	10.1	0.22	0.19	0.65	17.0	54.0
ER776	GF5	m-Cresol	H_2O_2	11.6	/	10.1	0.22	0.19	0.62	17.2	52.7

Table S2 Identified nitrogen-aromatic compounds by HPLC/ESI-Q-ToFMS from the oxidation of VOCs studied in this work.

Suggested Formula	Theoretical m/z $[M-H]^-$	Measured m/z $[M-H]^-$	Proposed structure[a]	Quantified as[b]	Absorbing as[c]
$C_6H_5NO_3$	138.0196	138.0199		 4-Nitrophenol ($C_6H_5NO_3$)	 4-Nitrophenol ($C_6H_5NO_3$)
$C_7H_7NO_3$	152.0353	152.0345		 2-Methyl-4-nitrophenol ($C_7H_7NO_3$)	 2-Methyl-4-nitrophenol ($C_7H_7NO_3$)
$C_6H_5NO_4$	154.0145	154.0146		 4-Nitrocatechol ($C_6H_5NO_4$)	 4-Nitrocatechol ($C_6H_5NO_4$)
$C_7H_7NO_4$	168.0302	168.0300		 2-Methyl-4-nitroresorcinol ($C_7H_7NO_4$)	 2-Methyl-4-nitroresorcinol ($C_7H_7NO_4$)
$C_6H_5NO_5$	170.0095	170.0094		 2-Nitrophloroglucinol ($C_6H_5NO_5$)	 2-Nitrophloroglucinol ($C_6H_5NO_5$)
$C_8H_7NO_4$	180.0302	180.0307		 2-Methyl-5-nitrobenzoic acid ($C_8H_7NO_4$)	 2-Methyl-5-nitrobenzoic acid ($C_8H_7NO_4$)

[a] Only one isomer of each formula was proposed for simplicity; [b] standard compounds used for the quantification of identified nitro-aromatic compounds; [c] standard compounds used to estimate the light absorption of quantified nitro-aromatic compounds.

Table S2. Continue.

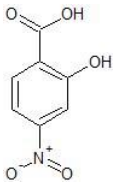
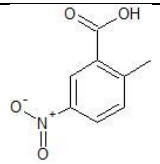
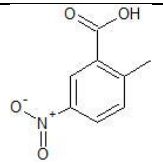
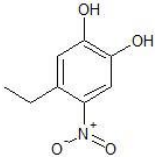
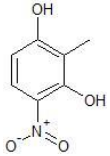
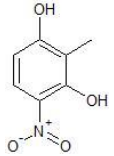
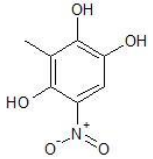
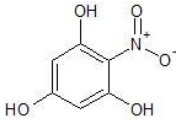
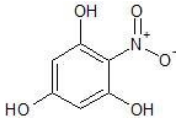
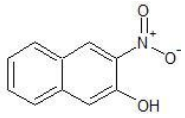
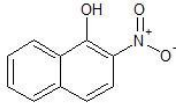
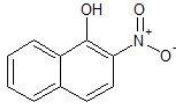
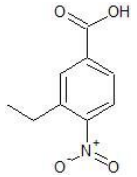
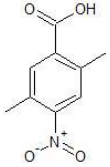
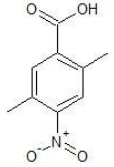
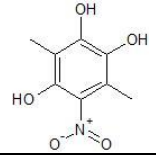
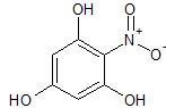
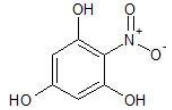
Suggested Formula	Theoretical m/z $[M-H]^-$	Measured m/z $[M-H]^-$	Proposed structure	Quantified as	Absorbing as
$C_7H_5NO_5$	182.0095	182.0098		 2-Methyl-5-nitrobenzoic acid ($C_8H_7NO_4$)	 2-Methyl-5-nitrobenzoic acid ($C_8H_7NO_4$)
$C_8H_9NO_4$	182.0459	182.0454		 2-Methyl-4-nitroresorcinol ($C_7H_7NO_4$)	 2-Methyl-4-nitroresorcinol ($C_7H_7NO_4$)
$C_7H_7NO_5$	184.0253	184.0255		 2-Nitrophloroglucinol ($C_6H_5NO_5$)	 2-Nitrophloroglucinol ($C_6H_5NO_5$)
$C_{10}H_7NO_3$	188.0353	188.0354		 2-Nitro-1-naphthol ($C_{10}H_7NO_3$)	 2-Nitro-1-naphthol ($C_{10}H_7NO_3$)
$C_9H_9NO_4$	194.0458	194.0459		 2,5-Dimethyl-4-nitrobenzoic acid ($C_9H_9NO_4$)	 2,5-Dimethyl-4-nitrobenzoic acid ($C_9H_9NO_4$)
$C_8H_9NO_5$	198.0407	198.0412		 2-Nitrophloroglucinol ($C_6H_5NO_5$)	 2-Nitrophloroglucinol ($C_6H_5NO_5$)

Table S2. Continue

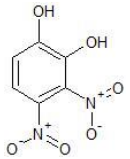
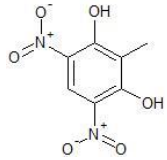
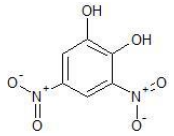
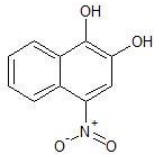
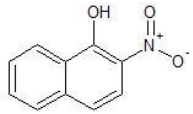
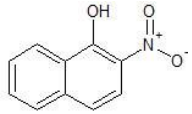
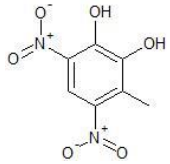
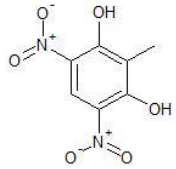
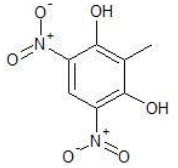
Suggested Formula	Theoretical m/z $[M-H]^-$	Measured m/z $[M-H]^-$	Proposed structure	Quantified as	Absorbing as
$C_6H_4N_2O_6$	198.9997	198.9994		 4,6-Dinitro-2-methylresorcinol ($C_7H_6N_2O_6$)	 3,5-Dinitrocatechol ($C_6H_4N_2O_6$)
$C_{10}H_7NO_4$	204.0302	204.0300		 2-Nitro-1-naphthol ($C_{10}H_7NO_3$)	 2-Nitro-1-naphthol ($C_{10}H_7NO_3$)
$C_7H_6N_2O_6$	213.0157	213.0149		 4,6-Dinitro-2-methylresorcinol ($C_7H_6N_2O_6$)	 4,6-Dinitro-2-methylresorcinol ($C_7H_6N_2O_6$)

Table S3 Recoveries and method detection limit (MDL) for standard compounds used for quantification.

Standard compounds	Formula	*m/z*, $[M-H]^-$	Recovery (N^a = 4, %)	Detection Limit (pg)
4-Nitrophenol	$C_6H_5NO_3$	138.0196	97.7 ± 0.92[b]	4.25
2-Methyl-4-nitrophenol	$C_7H_7NO_3$	152.0353	97.0 ± 0.78	2.31
4-Nitrocatechol	$C_6H_5NO_4$	154.0145	75.1 ± 0.48	4.79
2,6-Dimethyl-4-nitrophenol	$C_8H_9NO_3$	166.0510	100 ± 2.76	3.74
2-Methyl-4-nitroresocinol	$C_7H_7NO_4$	168.0302	105 ± 2.52	0.70
2-Nitrophloroglucinol	$C_6H_5NO_5$	170.0095	92.9 ± 7.10	2.55
2-Methyl-5-nitrobenzoic acid	$C_8H_7NO_4$	180.0302	106 ± 6.08	14.7
2-Nitro-1-naphthol	$C_{10}H_7NO_3$	188.0353	90.6 ± 6.56	16.1
2,5-dimethyl-4-nitrobenzoic acid	$C_9H_9NO_4$	194.0458	116 ± 4.52	17.6
4,6-Dinitro-2-methylresorcinol	$C_7H_6N_2O_6$	213.0157	113 ± 8.18	2.02

[a] Number of repetition; [b] mean ± standard deviation.

Table S4. Characteristics of linear regression between $A_{\lambda} - A_{700}$ and concentration of standard compounds.

Compounds	Formula	m/z, $[M-H]^-$	λ (nm)	Linear regression 1 (intercept = 0)			Linear regression 2 (intercept ≠ 0)			
				Conc. range (ng μL^{-1})[a]	MAE (m^2 g^{-1})[b]	*r*	Conc. range (ng μL^{-1})	MAE (m^2 g^{-1})	*b*[d]	*r*
4-Nitrophenol	$C_6H_5NO_3$	138.0196	365	< = 4.28	2.44	1.00				
			400	< = 1.07	0.71	0.94				
			450	/[c]	/	/				
			500	/	/	/				
			550	/	/	/				
2-Methyl-4-nitrophenol	$C_7H_7NO_3$	152.0353	365	< = 4.76	3.15	1.00				
			400	< = 1.19	0.53	0.71				
			450	/	/	/				
			500	/	/	/				
			550	/	/	/				
4-Nitrocatechol	$C_6H_5NO_4$	154.0145	365	< = 11.4	7.02	1.00				
			400	< 0.29	6.95	0.99	> = 0.29 and < = 11.4	2.39	1.61	1.00
			450	< 0.29	4.97	0.99	> = 0.29 and < = 11.4	1.11	1.36	1.00
			500	< 0.29	1.34	0.75	> = 0.29 and < = 11.4	0.18	0.21	0.96
			550	/	/	/				
2,6-Dimethyl-4-nitrophenol	$C_8H_9NO_3$	166.0510	365	< = 4.00	3.20	1.00				
			400	< = 4.00	0.51	0.99				
			450	/	/	/				
			500	/	/	/				
			550	/	/	/				
2-Methyl-4-nitroresorcinol	$C_7H_7NO_4$	168.0302	365	< = 33.3	12.9	1.00				
			400	< 1.11	4.49	0.99	> = 1.11 and < = 33.3	2.23	4.40	1.00
			450	< 1.11	1.20	0.97	> = 1.11 and < = 33.3	0.30	1.77	0.97
			500	/	/	/				
			550	/	/	/				
2-Nitrophloroglucinol	$C_6H_5NO_5$	170.0095	365	< = 3.72	14.0	1.00				
			400	< 0.93	14.1	1.00	> = 0.93 and < = 3.72	7.39	6.56	1.00
			450	< 0.93	1.61	0.99	> = 0.93 and < = 3.72	0.87	0.78	1.00
			500	/	/	/				
			550	/	/	/				

[a] Concentration ranges for linear relationship; [b] equals to slope × ln (10) × 100; [c] No absorption was observed at these wavelengths; [d] equals to intercept × ln (10) × 100.

Table S4. Continue

Compounds	Formula	MW	λ (nm)	Linear regression 1 (intercept = 0)			Linear regression 2 (intercept ≠ 0)			
				Conc. range (ng μL^{-1})	MAE (m^2 g^{-1})	*r*	Conc. range (ng μL^{-1})	MAE (m^2 g^{-1})	*b*	*r*
2-Methyl-5-nitrobenzoic acid	$C_8H_7NO_4$	180.0302	365	< = 2.14	0.35	0.93				
			400	/	/	/				
			450	/	/	/				
			500	/	/	/				
			550	/	/	/				
2-Nitro-1-naphthol	$C_{10}H_7NO_3$	188.0353	365	< = 4.64	3.75	1.00				
			400	< = 4.64	6.17	1.00				
			450	< = 4.64	2.33	1.00				
			500	< 1.16	0.39	0.97	> = 1.16 and < = 4.64	0.18	0.25	0.99
			550	/	/	/				
2,5-dimethyl-4-nitrobenzoic acid	$C_9H_9NO_4$	194.0458	365	< = 3.64	0.39	0.99				
			400	/	/	/				
			450	/	/	/				
			500	/	/	/				
			550	/	/	/				
3,5-Dinitrocatechol	$C_6H_4N_2O_6$	198.9997	365	< = 4.28	6.54	1.00				
			400	< = 4.28	7.00	0.99				
			450	< = 4.28	2.74	1.00				
			500	< = 4.28	0.58	0.98				
			550	< = 4.28	0.21	0.96				
4,6-Dinitro-2-methylresorcinol	$C_7H_6N_2O_6$	213.0153	365	< = 1.82	7.05	1.00				
			400	< = 1.82	11.4	1.00				
			450	< = 1.82	6.29	1.00				
			500	< = 1.82	0.32	0.97				
			550	/	/	/				

Table S5. Summary of average bulk MAE, *k* and $Å_a$ values of SOA extracts and their ranges for different chamber experiments.

	α-Pinene		Isoprene		β-Caryophyllene	
	NO_X (*N* = 4)	H_2O_2 (*N* = 2)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)	NO_X (*N* = 2)	H_2O_2 (*N* = 2)
λ (nm)			***MAE***			
365	0.026 ± 0.0058[a] (0.023 – 0.033)	0.019 ± 0.0023 (0.017 – 0.022)	NA	NA	0.010 ± 0.0092 (0.0010 – 0.019)	0.029 ± 0.011 (0.011 – 0.032)
400	0.018 ± 0.0071 (0.014 – 0.027)	0.0082 ± 0.0006 (0.076 – 0.0088)	NA	NA	NA	0.015 ± 0.0088 (0.0067 – 0.024)
450	0.0057 ± 0.0039 (0.0036 – 0.0098)	0.0037 ± 0.0005 (0.031 – 0.0042)	NA	NA	NA	0.0090 ± 0.0080 (0.0010 – 0.017)
500	NA[b]	NA	NA	NA	NA	0.0076 ± 0.011 (0.0000 – 0.015)
550	NA	NA	NA	NA	NA	0.0045 ± 0.0044 (0.0001 – 0.0089)
			k			
365	0.0009 ± 0.0002 (0.0008 – 0.0011)	0.0007 ± 0.0001 (0.0006 – 0.0008)	NA	NA	0.0004 ± 0.0003 (0.0000 – 0.007)	0.0008 ± 0.0004 (0.0004 – 0.0011)
400	0.0007 ± 0.0003 (0.0005 – 0.0010)	0.0003 ± 0.0000 (0.0003 – 0.0003)	NA	NA	NA	0.0006 ± 0.0003 (0.0003 – 0.0009)
450	0.0002 ± 0.0002 (0.0002 – 0.0004)	0.0002 ± 0.0000 (0.0001 – 0.0002)	NA	NA	NA	0.0004 ± 0.0003 (0.0000 – 0.0007)
500	NA	NA	NA	NA	NA	0.0004 ± 0.0004 (0.0000 – 0.0007)
550	NA	NA	NA	NA	NA	0.0002 ± 0.0002 (0.0000 – 0.0005)
			Absorption Angstrom Exponent calculation			
$Å_a$	15.3 ± 16.2 (8.51 – 39.5)	8.91 ± 0.19 (8.72 – 9.10)	33.0 ± 50.7 (2.73 – 91.5)	3.41 ± 0.68 (2.73 – 4.09)	14.8 ± 5.64 (9.15 – 20.4)	7.08 ± 3.66 (3.43 – 10.7)
r	-0.82 ± 0.19[c] (-0.88 – -0.55)	-0.92 ± 0.024 (-0.94 – -0.89)	-0.47 ± 0.21 (-0.68 – -0.24)	-0.57 ± 0.11 (-0.68 – -0.46)	-0.89 ± 0.06 (-0.95 – -0.83)	-0.96 ± 0.01 (-0.97 – -0.95)
% NA[d]	36.9 ± 43.1 (25.2 – 97.1)	16.9 ± 0.16 (16.7 – 17.2)	50.6 ± 42.3 (20.7 – 99.0)	84.6 ± 6.20 (78.4 – 90.8)	47.2 ± 26.2 (21.2 – 73.2)	14.0 ± 14.0 (0.00 – 28.0)

[a] For sample number *N* >2, represent mean ± standard deviation; for sample number *N*=2, represent mean ± difference/2; [b] 0 or very small negative values (close to 0) were obtained for these measurements; [c] correlation coefficients for the linear regression between log ($Abs_λ$) and log (λ), λ ranges from 300 to 550 nm; [d] represent the percentage of $A_λ$-A_{700} measurements with small negative values (close to 0) in the λ range of 300 to 550 nm; [e] significant difference ($p < 0.05$) has been observed for MAE values at 365 nm between NO_X and H_2O_2 conditions.

Table S5. Continue

	1,3,5-Trimethylbenzene		1,2,4-Trimethylbenzene		*m*-Xylene		Toluene[e]	
	NO_X (*N* = 2)	H_2O_2 (*N* = 2)	NO_X (*N* = 2)	H_2O_2 (*N* = 3)	NO_X (*N* = 4)	H_2O_2 (*N* = 5)	NO_X (*N* = 9)	H_2O_2 (*N* = 4)
λ (nm)				***MAE***				
365	NA	0.030 ± 0.019 (0.011 – 0.049)	0.17 ± 0.072 (0.094 – 0.24)	0.088 ± 0.018 (0.071 – 0.11)	0.12 ± 0.048 (0.094 – 0.19)	0.079 ± 0.016 (0.063 – 0.10)	0.55 ± 0.17 (0.39 – 0.96)	0.17 ± 0.051 (0.11 – 0.23)
400	NA	NA	0.082 ± 0.04 (0.042 – 0.12)	0.036 ± 0.0088 (0.027 – 0.45)	0.054 ± 0.023 (0.041 – 0.088)	0.033 ± 0.012 (0.021 – 0.052)	0.31 ± 0.093 (0.22 -0.53)	0.089 ± 0.031 (0.051 – 0.12)
450	NA	NA	0.032 ± 0.019 (0.013 – 0.051)	0.0065 ± 0.0029 (0.0042 – 0.0097)	0.014 ± 0.0071 (0.0091 – 0.024)	0.010 ± 0.010 (0.0014 – 0.027)	0.13 ± 0.036 (0.099 – 0.22)	0.033 ± 0.012 (0.016 – 0.042)
500	NA	NA	0.014 ± 0.0086 (0.0049 – 0.022)	NA	0.0038 ± 0.0034 (0.0011 – 0.0085)	0.0057 ± 0.0050 (0.0012 – 0.011)	0.052 ± 0.015 (0.035 – 0.085)	0.015 ± 0.0061 (0.0077 – 0.022)
550	NA	NA	0.0043 ± 0.0030 (0.013 – 0.73)	NA	0.0027 ± 0.0015 (0.0012 – 0.0042)	0.0050 ± 0.0052 (0.0006 – 0.011)	0.021 ± 0.0091 (0.0074 – 0.039)	0.0062 ± 0.0020 (0.0033 – 0.0076)
				K				
365	NA	0.0010 ± 0.0007 (0.0004 – 0.0017)	0.0058 ± 0.0025 (0.0033 – 0.0083)	0.0031 ± 0.0006 (0.0025 – 0.0037)	0.0042 ± 0.0017 (0.0033 – 0.0067)	0.0028 ± 0.0006 (0.0022 – 0.0035)	0.019 ± 0.0061 (0.014 – 0.034)	0.0060 ± 0.0018 (0.0038 – 0.0080)
400	NA	NA	0.0031 ± 0.0015 (0.0016 – 0.0046)	0.0014 ± 0.0003 (0.0010 – 0.0017)	0.0021 ± 0.0009 (0.0016 – 0.0033)	0.0013 ± 0.0005 (0.0008 – 0.0020)	0.012 ± 0.0035 (0.0086 – 0.020)	0.0034 ± 0.0012 (0.0019 – 0.0048)
450	NA	NA	0.0014 ± 0.0008 (0.0005 – 0.0022)	0.0003 ± 0.0001 (0.0002 – 0.0004)	0.0006 ± 0.0003 (0.0004 – 0.0010)	0.0004 ± 0.0004 (0.0001 – 0.0011)	0.0057 ± 0.0016 (0.0042 – 0.0093)	0.0014 ± 0.0005 (0.0007 – 0.0018)
500	NA	NA	0.0006 ± 0.0004 (0.0002 – 0.0011)	NA	0.0002 ± 0.0002 (0.0001 – 0.0004)	0.0003 ± 0.0002 (0.0001 – 0.0005)	0.0025 ± 0.0007 (0.0017 – 0.0041)	0.0007 ± 0.0003 (0.0004 – 0.0011)
550	NA	NA	0.0002 ± 0.0002 (0.01 – 0.0004)	NA	0.0001 ± 0.0001 (0.0001 – 0.0002)	0.0003 ± 0.0003 (0.0000 – 0.0006)	0.0011 ± 0.0005 (0.0004 – 0.0021)	0.0003 ± 0.0001 (0.0002 – 0.0004)
				Absorption Angstrom Exponent calculation				
$Å_a$	33.1 ± 26.0 (7.10 – 59.0)	15.1 ± 3.69 (11.4 – 18.8)	8.58 ± 1.29 (7.29 – 9.88)	11.9 ± 1.57 (10.1 – 13.0)	10.7 ± 1.69 (9.09 – 12.4)	10.1 ± 2.76 (6.17 – 12.8)	6.89 ± 0.63 (6.32 – 8.30)	7.69 ± 0.76 (6.96 – 8.74)
r	-0.93 ± 0.03 (-0.96 – -0.90)	-0.96 ± 0.00 (-0.96 – -0.95)	-0.98 ± 0.00 (-0.99 – -0.98)	-0.97 ± 0.01 (-0.97 – -0.96)	-0.97 ± 0.01 (-0.98 – -0.96)	-0.97 ± 0.02 (-0.99 – -0.95)	-0.99 ± 0.012 (-0.99 – -0.95)	-0.99 ± 0.01 (-1.00 – -0.98)
% NA	46.1 ± 46.0 (0.080 – 92.2)	39.2 ± 30.0 (9.19 – 69.2)	0.36 ± 0.28 (0.08 – 0.64)	18.3 ± 13.8 (2.40 – 26.8)	7.87 ± 6.18 (1.92 – 16.5)	9.88 ± 12.7 (0.00 – 29.1)	0.053 ± 0.16 (0.00 – 0.48)	0.00

Table S5. Continue

	Ethylbenzene[e]		Benzene[e]		Naphthalene[e]		*m*-Cresol[e]	
	NO_X (*N* = 6)	H_2O_2 (*N* = 5)	NO_X (*N* = 8)	H_2O_2 (*N* = 5)	NO_X (*N* = 3)	H_2O_2 (*N* = 3)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)
λ (nm)				***MAE***				
365	0.83 ± 0.26 (0.63 – 1.35)	0.32 ± 0.11 (0.15 – 0.43)	1.67 ± 0.66 (1.12 – 2.79)	0.36 ± 0.066 (0.31 – 0.45)	1.17 ± 0.088 (1.07 – 1.23)	0.62 ± 0.027 (0.60 – 0.65)	2.47 ± 1.05 (1.30 – 3.26)	0.24 ± 0.0003 (0.24 – 0.24)
400	0.50 ± 0.14 (0.36 – 0.77)	0.18 ± 0.076 (0.070 – 0.25)	0.88 ± 0.21 (0.70 – 1.28)	0.21 ± 0.048 (0.17 – 0.27)	0.78 ± 0.074 (0.70 – 0.84)	0.35 ± 0.028 (0.33 – 0.38)	1.19 ± 0.37 (0.78 – 1.50)	0.11 ± 0.0009 (0.11 – 0.12)
450	0.22 ± 0.061 (0.14 – 0.33)	0.078 ± 0.039 (0.021 – 0.12)	0.41 ± 0.064 (0.34 – 0.53)	0.097 ± 0.031 (0.068 – 0.13)	0.43 ± 0.034 (0.40 – 0.46)	0.17 ± 0.017 (0.15 – 0.19)	0.39 ± 0.056 (0.34 – 0.45)	0.043 ± 0.0015 (0.041 – 0.044)
500	0.093 ± 0.026 (0.057 – 0.14)	0.034 ± 0.020 (0.0058 – 0.057)	0.19 ± 0.032 (0.16 – 0.25)	0.042 ± 0.017 (0.023 – 0.060)	0.25 ± 0.015 (0.23 – 0.26)	0.081 ± 0.0098 (0.073 – 0.092)	0.17 ± 0.033 (0.15 – 0.21)	0.017 ±0.0029 (0.014 – 0.020)
550	0.039 ± 0.013 (0.021 – 0.057)	0.011 ± 0.0093 (0.0003 – 0.023)	0.087 ± 0.015 (0.071 – 0.12)	0.017 ± 0.0085 (0.0068 – 0.025)	0.12 ± 0.011 (0.11 – 0.13)	0.037 ± 0.0078 (0.033 – 0.046)	0.077 ± 0.014 (0.067 – 0.093)	0.0087 ± 0.0007 (0.0080 – 0.0094)
				K				
365	0.029 ± 0.0091 (0.022 – 0.047)	0.011 ± 0.0039 (0.0053 – 0.015)	0.058 ± 0.023 (0.039 – 0.097)	0.013 ± 0.0023 (0.011 – 0.016)	0.041 ± 0.0031 (0.037 – 0.043)	0.022 ± 0.0009 (0.021 – 0.023)	0.086 ± 0.037 (0.045 – 0.11)	0.0083 ± 0.0000 (0.0083 – 0.0084)
400	0.019 ± 0.0054 (0.014 – 0.030)	0.0069 ± 0.0029 (0.0027 – 0.0097)	0.034 ± 0.0080 (0.027 – 0.049)	0.0082 ± 0.0018 (0.0065 – 0.010)	0.030 ± 0.0028 (0.027 – 0.032)	0.013 ± 0.0011 (0.013 – 0.015)	0.045 ± 0.014 (0.030 – 0.057)	0.0044 ± 0.0000 (0.0043 – 0.0044)
450	0.0096 ± 0.0026 (0.0060 – 0.014)	0.0034 ± 0.0017 (0.0009 – 0.0051)	0.017 ± 0.0027 (0.015 – 0.023)	0.0042 ± 0.0013 (0.0029 – 0.0057)	0.019 ± 0.0015 (0.017 – 0.020)	0.0072 ± 0.0007 (0.0066 – 0.0080)	0.017 ± 0.0024 (0.015 – 0.019)	0.0018 ± 0.0001 (0.0018 – 0.0019)
500	0.0044 ± 0.0012 (0.0027 – 0.0065)	0.0016 ± 0.0009 (0.0003 – 0.0027)	0.0090 ± 0.0015 (0.0076 – 0.012)	0.0020 ± 0.0008 (0.0011 – 0.0029)	0.012 ± 0.0007 (0.011 – 0.013)	0.0039 ± 0.0005 (0.0035 – 0.0044)	0.0081 ± 0.0016 (0.0070 – 0.0099)	0.0008 ± 0.0001 (0.0007 – 0.0010)
550	0.0020 ± 0.0007 (0.0011 – 0.0030)	0.0006 ± 0.0005 (0.0000 – 0.0012)	0.0046 ± 0.0008 (0.0038 – 0.0061)	0.0009 ± 0.0004 (0.0004 – 0.0013)	0.0062 ± 0.0006 (0.0058 – 0.0069)	0.0020 ± 0.0004 (0.0017 – 0.0024)	0.0040 ± 0.0007 (0.0035 – 0.0049)	0.0005 ± 0.0000 (0.0004 – 0.0005)
				Absorption Angstrom Exponent calculation				
$Å_a$	6.39 ± 0.44 (5.80 – 7.09)	7.46 ± 1.32 (6.29 – 9.64)	5.84 ± 0.50 (5.24 – 6.63)	6.53 ± 0.72 (5.88 – 7.45)	4.92 ± 0.23 (4.71 – 5.16)	6.46 ± 0.25 (6.17 – 6.63)	6.86 ± 0.97 (5.82 – 7.70)	7.75 ± 0.24 (7.51 – 7.99)
r	-0.99 ± 0.00 (-0.99 – -0.98)	-0.99 ± 0.00 (-0.99 - -0.99)	-0.98 ± 0.00 (-0.98 - -0.98)	-0.99 ± 0.00 (-0.99 - -0.99)	-1.00 ± 0.00 (-1.00 – -0.99)	-1.00 ± 0.00 (-1.00 – -1.00)	-0.98 ± 0.01 (-0.98 – -0.96)	-1.00 ± 0.00 (-1.00 – -1.00)
% NA	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S6. Average and ranges of mass contribution (%) of identified nitro-aromatic compounds to SOA generated from chamber experiments.

Suggested Formula	m/z $[M-H]^-$ [a]	*α*-Pinene		Isoprene		*β*-Caryophyllene	
		NO_X (N = 4)	H_2O_2 (N = 2)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)	NO_X (N = 2)	H_2O_2 (N = 2)
$C_6H_5NO_3$	138.0196	/[b]	/	/	/	/	/
$C_7H_7NO_3$	152.0353	0.0020 ± 0.0013[c] (0.0008 – 0.0038)	/	/	/	0.0020 ± 0.0005 (0.0014 – 0.0025)	/
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/
$C_7H_7NO_4$	168.0302	0.0024 ± 0.0019 (0.0007 – 0.0044)	0.0009 ± 0.0001 (0.0009 – 0.0010)	0.0089 ± 0.0083 (0.0031 – 0.015)	/	0.0072 ± 0.0051 (0.0021 – 0.012)	/
$C_6H_5NO_5$	170.0095	0.0078 ± 0.0022 (0.0059 – 0.010)	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	/	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/

[a] The mass accuracy for all identified formula are within 10 ppm; [b] not detected; [c] for sample number *N* >2, represent mean ± standard deviation; for sample number *N*=2, represent mean ± difference/2;

Table S6. Continue

Suggested formula	m/z $[M-H]^-$	1,3,5-Trimethylbenzene		1,2,4-Trimethylbenzene		*m*-Xylene		Toluene	
		NO_X (N = 2)	H_2O_2 (N = 3)	NO_X (N = 2)	H_2O_2 (N = 3)	NO_X (*N* = 4)	H_2O_2 (*N* = 5)	NO_X (*N* = 9)	H_2O_2 (*N* = 4)
$C_6H_5NO_3$	138.0196	/	/	/	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	0.0019 ± 0.0001 (0.0019 – 0.0020)	/	0.0021 ± 0.0001 (0.0021 – 0.0022)	/	0.030 ± 0.010 (0.014 – 0.045)	0.0034 ± 0.0035 (0.0010 – 0.0074)
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/	0.088 ± 0.036 (0.052 – 0.17)	0.0028 ± 0.0011 (0.0017 – 0.0038)
$C_7H_7NO_4$	168.0302	/	/	0.012 ± 0.0078 (0.0044 – 0.020)	/	0.010 ± 0.0098 (0.0030 – 0.025)	/	0.29 ± 0.17 (0.082 – 0.62)	0.012 ± 0.016 (0.0022 – 0.030)
$C_6H_5NO_5$	170.0095	/	/	/	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	0.11 ± 0.0067 (0.10 – 0.12)	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	0.011 ± 0.0030 (0.0075 – 0.014)	/	0.019 ± 0.0035 (0.016 – 0.024)	0.0006 ± 0.0001 (0.0006 – 0.0008)	0.0053 ± 0.0026 (0.0032 – 0.010)	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/	0.030 ± 0.011 (0.014 – 0.044)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	0.062 ± 0.031 (0.031 – 0.092)		0.0085 ± 0.0033 (0.0049 – 0.013)	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	0.0032 ± 0.0011 (0.0025 – 0.0045)	/	0.0076 ± 0.0034 (0.0032 – 0.013)	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	0.19 ± 0.093 (0.072 – 0.34)	/

Table S6. Continue

Suggested formula	m/z $[M-H]^-$	Ethylbenzene		Benzene		Naphthalene		*m*-Cresol	
		NO_X (N = 6)	H_2O_2 (N =5)	NO_X (N = 8)	H_2O_2 (N =5)	NO_X (*N* = 3)	H_2O_2 (*N* = 3)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	0.0048 ± 0.0020 (0.0030 – 0.0078)	/	0.0068 ± 0.0046 (0.0024 – 0.013)	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	/	/	0.0083 ± 0.0015 (0.0073 – 0.0094)	/	0.062 ± 0.051 (0.027 – 0.12)	/
$C_6H_5NO_4$	154.0145	0.23 ± 0.10 (0.15 – 0.40)	0.012 ± 0.0036 (0.0076 – 0.017)	4.65 ± 3.78 (1.05 – 12.0)	0.051 ± 0.043 (0.020 – 0.12)	0.094 ± 0.090 (0.039 – 0.20)	/	0.055 ± 0.017 (0.036 -0.069)	/
$C_7H_7NO_4$	168.0302	0.0054 ± 0.0048 (0.0015 – 0.013)	/	/	/	0.0060 ± 0.0038 (0.0023 – 0.0099)	/	8.34 ± 5.87 (3.03 – 14.6)	/
$C_6H_5NO_5$	170.0095	0.0079 ± 0.0029 (0.0044 – 0.012)	/	1.08 ± 0.39 (0.64 – 1.71)	/	/	/	0.016 ± 0.0079 (0.011 – 0.022)	/
$C_8H_7NO_4$	180.0302	0.27 ± 0.21 (0.12 – 0.62)	/	/	/	0.47 ± 0.39 (0.075 – 0.85)	/	0.20 ± 0.12 (0.12 – 0.29)	/
$C_7H_5NO_5$	182.0095	0.21 ± 0.095 (0.11 – 0.33)	/	/	/	0.26 ± 0.076 (0.19 – 0.34)	/	/	/
$C_8H_9NO_4$	182.0459	0.32 ± 0.26 (0.16 – 0.78)	/	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	0.015 ± 0.0069 (0.0056 – 0.026)	/	/	/	1.43 ± 0.69 (0.84 – 2.19)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	4.05 ± 1.37 (3.20 – 5.63)	1.37 ± 1.55 (0.43 – 3.16)	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	0.052 ± 0.028 (0.032 – 0.10)	/	/	/	0.14 ± 0.089 (0.041 – 0.22)	/	0.21 ± 0.083 (0.11 – 0.27)	/
$C_6H_4N_2O_6$	198.9997	/	/	0.045 ± 0.039 (0.014 – 0.13)	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	1.39 ± 0.37 (1.06 – 1.79)	0.25 ± 0.28 (0.085 – 0.58)	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	0.032 ± 0.019 (0.018 – 0.054)	/

Table S7. Average and ranges of contribution (%) of identified nitro-aromatic compounds to light absorption at 365 nm (Abs_{365}) of SOA generated from chamber experiments.

Suggested formula	m/z $[M-H]^-$	*α*-Pinene		Isoprene		*β*-Caryophyllene	
		NO_X (*N* = 4)	H_2O_2 (*N* = 2)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)	NO_X (*N* = 2)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	/[a]	/	/	/	/	/
$C_7H_7NO_3$	152.0353	0.29 ± 0.23[b] (0.11 – 0.55)	/	/	/	2.42 ± 2.01 (0.41 – 4.43)	/
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/
$C_7H_7NO_4$	168.0302	1.10 ±1.31 (0.28 – 2.60)	0.64 ± 0.13 (0.51 – 0.77)	/	/	/	/
$C_6H_5NO_5$	170.0095	4.65 ±1.84 (3.41 – 6.76)	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	/	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/

[a] No absorption could be estimated, since the compound could not be detected or the compound has no absorption at the given wavelength (λ); [b] for sample number *N* >2, represent mean ± standard deviation; for sample number *N*=2, represent mean ± difference/2.

Table S7. Continue

Suggested formula	m/z $[M-H]^-$	1,3,5-Trimethylbenzene		1,2,4-Trimethylbenzene		*m*-Xylene		Toluene	
		NO_X (N = 2)	H_2O_2 (N = 3)	NO_X (N = 2)	H_2O_2 (N = 3)	NO_X (*N* = 4)	H_2O_2 (*N* = 5)	NO_X (*N* = 9)	H_2O_2 (*N* = 4)
$C_6H_5NO_3$	138.0196	/	/	/	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	0.045 ± 0.018 (0.027 – 0.063)	/	0.069 ± 0.0007 (0.068 – 0.070)	/	0.18 ± 0.081 (0.10 – 0.33)	0.050 ± 0.045 (0.020 – 0.10)
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/	1.12 ± 0.20 (0.92 – 1.56)	0.13 ± 0.037 (0.10 – 0.17)
$C_7H_7NO_4$	168.0302	/	/	0.85 ± 0.24 (0.61 – 1.09)	/	0.92 ± 0.52 (0.39 – 1.64)	/	6.68 ± 3.09 (2.73 – 11.2)	0.72 ± 0.84 (0.15 – 1.69)
$C_6H_5NO_5$	170.0095	/	/	/	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	0.28 ± 0.11 (0.17 – 0.38)	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	0.88 ± 0.15 (0.74 – 1.03)	/	2.08 ± 0.38 (1.58 – 2.41)	0.12 ± 0.035 (0.088 – 0.16)	0.12 ± 0.052 (0.078 – 0.21)	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/	0.77 ± 0.28 (0.49 – 1.36)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	0.14 ± 0.011 (0.13 – 0.15)	/	0.028 ± 0.0073 (0.021 – 0.038)	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	0.36 ± 0.032 (0.32 – 0.39)	/	0.19 ± 0.071 (0.12 – 0.35)	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	2.43 ± 1.08 (1.31 – 4.55)	/

Table S7. Continue

Suggested formula	m/z $[M-H]^-$	Ethylbenzene		Benzene		Naphthalene		*m*-Cresol	
		NO_X (N = 6)	H_2O_2 (N =5)	NO_X (N = 8)	H_2O_2 (N =5)	NO_X (*N* = 3)	H_2O_2 (*N* = 3)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	0.014 ± 0.0059 (0.0094 – 0.025)	/	0.0090 ± 0.0050 (0.0045 – 0.019)	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	/	/	0.023 ± 0.0022 (0.021 – 0.024)	/	0.075 ± 0.038 (0.041 – 0.12)	/
$C_6H_5NO_4$	154.0145	1.91 ± 0.52 (1.17 – 2.57)	0.27 ± 0.069 (0.20 – 0.35)	17.5 ± 9.28 (6.53 – 33.0)	1.07 ± 1.01 (0.32 – 2.62)	0.55 ± 0.50 (0.23 – 1.12)	/	0.20 ± 0.16 (0.078 – 0.38)	/
$C_7H_7NO_4$	168.0302	0.074 ± 0.047 (0.024 – 0.13)	/	/	/	0.067 ± 0.041 (0.024 – 0.11)	/	40.5 ± 15.2 (30.6 – 57.9)	/
$C_6H_5NO_5$	170.0095	0.13 ± 0.054 (0.082 – 0.21)	/	10.1 ± 4.22 (3.22 – 15.5)	/	/	/	0.14 ± 0.14 (0.045 – 0.24)	/
$C_8H_7NO_4$	180.0302	0.11 ± 0.079 (0.051 – 0.25)	/	/	/	0.15 ± 0.13 (0.021 – 0.28)	/	0.023 ± 0.011 (0.015 – 0.031)	/
$C_7H_5NO_5$	182.0095	0.082 ± 0.023 (0.048 – 0.10)	/	/	/	0.077 ± 0.021 (0.055 – 0.096)	/	/	/
$C_8H_9NO_4$	182.0459	4.53 ± 2.38 (1.52 – 7.46)	/	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	0.14 ± 0.063 (0.048 – 0.24)	/	/	/	8.25 ± 1.79 (6.19 – 9.41)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	13.2 ± 5.62 (9.74 – 19.7)	8.09 ± 8.84 (2.62 – 18.3)	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	0.84 ± 0.26 (0.54 – 1.13)	/	/	/	1.7 ± 1.18 (0.46 – 2.82)	/	1.18 ± 0.17 (0.99 – 1.33)	/
$C_6H_4N_2O_6$	198.9997	/	/	0.17 ± 0.17 (0.040 – 0.54)	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	4.52 ±1.56 (3.22 – 6.25)	1.49 ± 1.61 (0.51 – 3.35)	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	0.094 ± 0.040 (0.053 – 0.13)	/

Table S8. Average and ranges of contribution (%) of identified nitro-aromatic compounds to light absorption at 400 nm (Abs_{400}) of SOA generated from chamber experiments.

Suggested formula	m/z $[M-H]^-$	*α*-Pinene		Isoprene		*β*-Caryophyllene	
		NO_X (*N* = 4)	H_2O_2 (*N* = 2)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)	NO_X (*N* = 2)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	/[a]	/	/	/	/	/
$C_7H_7NO_3$	152.0353	0.072 ± 0.059[b] (0.031 – 0.14)	/	/	/	/	/
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/
$C_7H_7NO_4$	168.0302	0.57 ± 0.68 (0.12 – 1.35)	0.51 ± 0.0063 (0.50 – 0.51)	/	/	/	/
$C_6H_5NO_5$	170.0095	6.88 ± 2.87 (4.66 – 10.1)	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	/	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/

[a] No absorption could be estimated, since the compound could not be detected or the compound has no absorption at the given wavelength (λ); [b] for sample number *N* >2, represent mean ± standard deviation; for sample number *N*=2, represent mean ± difference/2.

Table S8. Continue

Suggested formula	m/z $[M-H]^-$	1,3,5-Trimethylbenzene		1,2,4-Trimethylbenzene		m-Xylene		Toluene	
		NO_X (*N* = 2)	H_2O_2 (*N* = 3)	NO_X (*N* = 2)	H_2O_2 (*N* = 3)	NO_X (*N* = 4)	H_2O_2 (*N* = 5)	NO_X (*N* = 9)	H_2O_2 (*N* = 4)
$C_6H_5NO_3$	138.0196	/	/	/	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	0.016 ± 0.0076 (0.0087 – 0.024)	/	0.027 ± 0.0015 (0.025 – 0.028)	/	0.055 ± 0.025 (0.030 – 0.10)	0.016 ± 0.014 (0.0063 – 0.032)
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/	1.96 ± 0.40 (1.55 – 2.78)	0.25 ± 0.061 (0.20 – 0.32)
$C_7H_7NO_4$	168.0302	/	/	0.61 ± 0.13 (0.43 – 0.74)	/	0.72 ± 0.40 (0.32 – 1.26)	/	4.10 ± 1.94 (1.65 – 7.01)	0.47 ± 0.54 (0.10 – 1.09)
$C_6H_5NO_5$	170.0095	/	/	/	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	0.65 ± 0.15 (0.50 – 0.81)	/	1.65 ± 0.32 (1.21 – 1.96)	0.11 ± 0.036 (0.067 – 0.13)	0.076 ± 0.035 (0.043 – 0.13)	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/	1.36 ± 0.49 (0.85 – 2.33)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	0.80 ± 0.080 (0.72 – 0.87)	/	0.34 ± 0.12 (0.20 – 0.60)	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	6.90 ± 3.06 (3.68 – 12.4)	/

Table S8. Continue

Suggested formula	m/z $[M-H]^-$	Ethylbenzene		Benzene		Naphthalene		*m*-Cresol	
		NO_X (*N* = 6)	H_2O_2 (*N* =5)	NO_X (N = 8)	H_2O_2 (N =5)	NO_X (*N* = 3)	H_2O_2 (*N* = 3)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	0.0070 ± 0.0032 (0.0044 – 0.013)	/	0.0050 ± 0.0030 (0.0022 – 0.010)	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	/	/	0.0058 ± 0.0004 (0.0055 – 0.0061)	/	0.026 ± 0.015 (0.015 – 0.043)	/
$C_6H_5NO_4$	154.0145	3.10 ± 0.83 (2.04 – 4.18)	0.50 ± 0.17 (0.34 – 0.75)	17.9 ± 6.57 (10.5 – 29.8)	1.88 ± 1.84 (0.53 – 4.71)	0.80 ± 0.73 (0.33 – 1.64)	/	0.37 ± 0.23 (0.17 – 0.62)	/
$C_7H_7NO_4$	168.0302	0.044 ± 0.029 (0.013 – 0.076)	/	/	/	0.035 ± 0.021 (0.012 – 0.054)	/	21.7 ± 3.73 (17.4 – 24.1)	/
$C_6H_5NO_5$	170.0095	0.21 ± 0.082 (0.13 – 0.34)	/	18.0 ± 6.80 (7.09 – 28.6)	/	/	/	0.25 ± 0.21 (0.099 – 0.39)	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	2.59 ± 1.39 (0.93 – 4.54)	/	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	0.25 ± 0.11 (0.11 – 0.41)	/	/	/	14.2 ± 0.80 (13.6 – 15.1)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	32.8 ± 14.7 (23.7 – 49.7)	22.9 ± 24.3 (7.77 – 50.9)	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	1.39 ± 0.41 (0.96 – 1.83)	/	/	/	2.61 ± 1.84 (0.69 – 4.36)	/	2.40 ± 0.52 (2.04 – 3.00)	/
$C_6H_4N_2O_6$	198.9997	/	/	0.34 ± 0.33 (0.10 – 1.06)	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	11.2 ± 4.11 (7.84 – 15.8)	4.22 ± 4.42 (1.52 – 9.32)	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	0.31 ± 0.15 (0.19 – 0.48)	/

Table S9. Average and ranges of contribution (%) of identified nitro-aromatic compounds to light absorption at 450 nm (Abs_{450}) of SOA generated from chamber experiments.

Suggested formula	m/z $[M-H]^-$	*α*-Pinene		Isoprene		*β*-Caryophyllene	
		NO_X (*N* = 4)	H_2O_2 (*N* = 2)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)	NO_X (*N* = 2)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	/[a]	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	/	/	/	/
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/
$C_7H_7NO_4$	168.0302	0.15 ± 0.18[b] (0.031 – 0.36)	0.14 ± 0.0017 (0.13 – 0.14)	/	/	/	/
$C_6H_5NO_5$	170.0095	0.79 ± 0.33 (0.53 – 1.16)	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	/	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/

[a] No absorption could be estimated, since the compound could not be detected or the compound has no absorption at the given wavelength (λ); [b] for sample number *N* >2, represent mean ± standard deviation; for sample number *N*=2, represent mean ± difference/2.

Table S9. Continue

Suggested formula	m/z $[M-H]^-$	1,3,5-Trimethylbenzene		1,2,4-Trimethylbenzene		*m*-Xylene		Toluene	
		NO_X (*N* = 2)	H_2O_2 (*N* = 3)	NO_X (*N* = 2)	H_2O_2 (*N* = 3)	NO_X (*N* = 4)	H_2O_2 (*N* = 5)	NO_X (*N* = 9)	H_2O_2 (*N* = 4)
$C_6H_5NO_3$	138.0196	/	/	/	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	/	/	/	/	/	/
$C_6H_5NO_4$	154.0145	/	/	/	/	/	/	1.40 ± 0.29 (1.11 – 1.99)	0.18 ± 0.044 (0.14 – 0.23)
$C_7H_7NO_4$	168.0302	/	/	0.16 ± 0.035 (0.13 – 0.20)	/	0.19 ± 0.11 (0.085 – 0.34)	/	1.10 ± 0.52 (0.44 – 1.87)	0.12 ± 0.14 (0.027 – 0.29)
$C_6H_5NO_5$	170.0095	/	/	/	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	0.17 ± 0.041 (0.13 – 0.22)	/	0.44 ± 0.085 (0.32 – 0.52)	0.029 ± 0.0095 (0.018 – 0.036)	0.020 ± 0.0095 (0.011 – 0.036)	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/	0.16 ± 0.056 (0.097 – 0.27)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	0.092 ± 0.0091 (0.082 – 0.10)	/	0.039 ± 0.014 (0.023 – 0.069)	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	3.80 ± 1.69 (2.03 – 6.82)	/

Table S9. Continue

Suggested formula	m/z $[M-H]^-$	Ethylbenzene		Benzene		Naphthalene		*m*-Cresol	
		NO_X (*N* = 6)	H_2O_2 (*N* = 5)	NO_X (*N* = 8)	H_2O_2 (*N* = 5)	NO_X (*N* = 3)	H_2O_2 (*N* = 3)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	/	/	/	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	/	/	/	/	/	/
$C_6H_5NO_4$	154.0145	2.22 ± 0.59 (1.46 – 2.99)	0.36 ± 0.12 (0.24 – 0.54)	10.7 ± 3.22 (7.50 – 15.0)	1.34 ± 1.31 (0.38 – 3.37)	0.58 ± 0.52 (0.24 – 1.17)	/	0.26 ± 0.16 (0.12 – 0.44)	/
$C_7H_7NO_4$	168.0302	0.012 ± 0.0078 (0.0036 – 0.020)	/	/	/	0.0093 ± 0.0057 (0.0033 – 0.015)	/	4.87 ± 1.32 (3.68 – 6.30)	/
$C_6H_5NO_5$	170.0095	0.024 ± 0.0093 (0.015 – 0.039)	/	2.05 ± 0.78 (0.81 – 3.27)	/	/	/	0.028 ± 0.024 (0.011 – 0.045)	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	0.69 ± 0.37 (0.25 – 1.21)	/	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	0.029 ± 0.012 (0.012 – 0.047)	/	/	/	1.64 ± 0.073 (1.50 – 1.73)	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	12.4 ± 5.55 (8.93 – 18.8)	8.64 ± 9.18 (2.93 – 19.2)	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	0.16 ± 0.047 (0.11 – 0.21)	/	/	/	0.30 ± 0.21 (0.079 – 0.50)	/	0.27 ± 0.059 (0.23 – 0.34)	/
$C_6H_4N_2O_6$	198.9997	/	/	0.13 ± 0.13 (0.040 – 0.41)	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	4.23 ± 1.55 (2.96 – 5.96)	1.59 ± 1.67 (0.58 – 3.52)	/	/
$C_7H_6N_2O_6$	213.0157	/	/	/	/	/	/	0.17 ± 0.084 (0.10 – 0.26)	/

Table S10. Average and ranges of contribution (%) of identified nitro-aromatic compounds to light absorption at 500 nm (Abs_{500}) of SOA generated from chamber experiments.

Suggested formula	MW [M-H]-	Toluene		Ethylbenzene		Benzene		Naphthalene		*m*-Cresol	
		NO_X (*N* = 9)	H_2O_2 (*N* = 4)	NO_X (*N* = 6)	H_2O_2 (*N* = 5)	NO_X (*N* = 8)	H_2O_2 (*N* = 5)	NO_X (*N* = 3)	H_2O_2 (*N* = 3)	NO_X (*N* = 3)	H_2O_2 (*N* = 2)
$C_6H_5NO_3$	138.0196	/[a]	/	/	/	/	/	/	/	/	/
$C_7H_7NO_3$	152.0353	/	/	/	/	/	/	/	/	/	/
$C_6H_5NO_4$	154.0145	0.38 ± 0.078[b] (0.30 – 0.54)	0.048 ± 0.012 (0.038 – 0.061)	0.60 ± 0.16 (0.066 – 0.15)	0.097 ± 0.034 (0.39 – 0.81)	2.11 ± 0.79 (1.22 – 3.80)	0.36 ± 0.35 (0.10 – 0.91)	0.16 ± 0.14 (0.064 – 0.32)	/	0.071 ± 0.044 (0.033 – 0.12)	/
$C_7H_7NO_4$	168.0302	/	/	/	/	/	/	/	/	/	/
$C_6H_5NO_5$	170.0095	/	/	/	/	/	/	/	/	/	/
$C_8H_7NO_4$	180.0302	/	/	/	/	/	/	/	/	/	/
$C_7H_5NO_5$	182.0095	/	/	/	/	/	/	/	/	/	/
$C_8H_9NO_4$	182.0459	/	/	/	/	/	/	/	/	/	/
$C_7H_7NO_5$	184.0253	/	/	/	/	/	/	/	/	/	/
$C_{10}H_7NO_3$	188.0353	/	/	/	/	/	/	2.07 ± 0.93 (1.50 -3.14)	1.36 ± 1.38 (0.49 – 2.96)	/	/
$C_9H_9NO_4$	194.0458	/	/	/	/	/	/	/	/	/	/
$C_8H_9NO_5$	198.0407	/	/	/	/	/	/	/	/	/	/
$C_6H_4N_2O_6$	198.9997	/	/	/	/	0.028 ± 0.028 (0.0085 – 0.088)	/	/	/	/	/
$C_{10}H_7NO_4$	204.0302	/	/	/	/	/	/	0.71 ± 0.26 (0.50 -1.00)	0.27 ± 0.28 (0.096 – 0.60)	/	/
$C_7H_6N_2O_6$	213.0157	0.19 ± 0.086 (0.10 – 0.35)	/	/	/	/	/	/	/	0.0087 ± 0.0043 (0.0052 – 0.013)	/

[a] No absorption could be estimated, since the compound could not be detected or the compound has no absorption at the given wavelength (λ); [b] for sample number *N* >2, represent mean ± standard deviation; for sample number *N*=2, represent mean ± difference/2.

Table S11. Average and ranges of contribution (%) of identified nitro-aromatic compounds to light absorption at 550 nm (Abs_{550}) of SOA generated from chamber experiments.

Suggested formula	MW $[M-H]^-$	Benzene	
		NO_X (*N* = 8)	H_2O_2 (*N* = 5)
$C_6H_5NO_3$	138.0196	/[a]	/
$C_7H_7NO_3$	152.0353	/	/
$C_6H_5NO_4$	154.0145	/	/
$C_7H_7NO_4$	168.0302	/	/
$C_6H_5NO_5$	170.0095	/	/
$C_8H_7NO_4$	180.0302	/	/
$C_7H_5NO_5$	182.0095	/	/
$C_8H_9NO_4$	182.0459	/	/
$C_7H_7NO_5$	184.0253	/	/
$C_{10}H_7NO_3$	188.0353	/	/
$C_9H_9NO_4$	194.0458	/	/
$C_8H_9NO_5$	198.0407	/	/
$C_6H_4N_2O_6$	198.9997	0.010 ± 0.010[b] (0.0031 – 0.032)	/
$C_{10}H_7NO_4$	204.0302	/	/
$C_7H_6N_2O_6$	213.0157	/	/

[a] No absorption could be estimated, since the compound could not be detected or the compound has no absorption at the given wavelength (λ); [b] for sample number *N* >2, represent mean ± standard deviation; for sample number *N*=2, represent mean ± difference/2.

Table S12. Average MAE differences ($m^2 g^{-1}$) between NO_X and H_2O_2 reaction conditions derived from sample extracts and contributions of nitro-aromatic compounds.

VOCs	365 nm			400 nm			450 nm		
	Bulk[a]	Species[b]	S/B (%)[c]	Bulk	Species	S/B (%)	Bulk	Species	S/B (%)
1,3,5-Trimethylbenzene	0.017	/[d]	/	0.0064	/	/	0.011	/	/
1,2,4-Trimethylbenzene	0.078	0.0036	4.66	0.080	0.0010	1.28	0.045	0.0003	0.60
m-Xylene	0.043	0.0041	9.60	0.055	0.0020	3.57	0.021	0.0006	2.66
Toluene	0.37	0.062	16.7	0.44	0.046	10.31	0.22	0.020	9.15
Ethylbenzene	0.51	0.067	13.1	0.60	0.039	6.39	0.32	0.016	4.96
Benzene	1.31	0.48	36.7	1.51	0.32	21.0	0.67	0.11	16.6
Naphthalene	0.55	0.17	31.1	0.59	0.26	44.1	0.43	0.096	22.1
m-Cresol	2.23	1.32	59.0	2.41	0.47	19.6	1.07	0.085	7.93

[a] Difference of average bulk MAE value of sample extracts between NO_X and H_2O_2 reactions; [b] difference of average MAE contributed by identified nitro-aromatic compounds between NO_X and H_2O_2 reactions; [c] species/bulk × 100%, the differences of MAE in sample extracts accounted for by that in contributions from nitro-aromatic compounds; [d] no nitro-aromatic compounds has been detected.

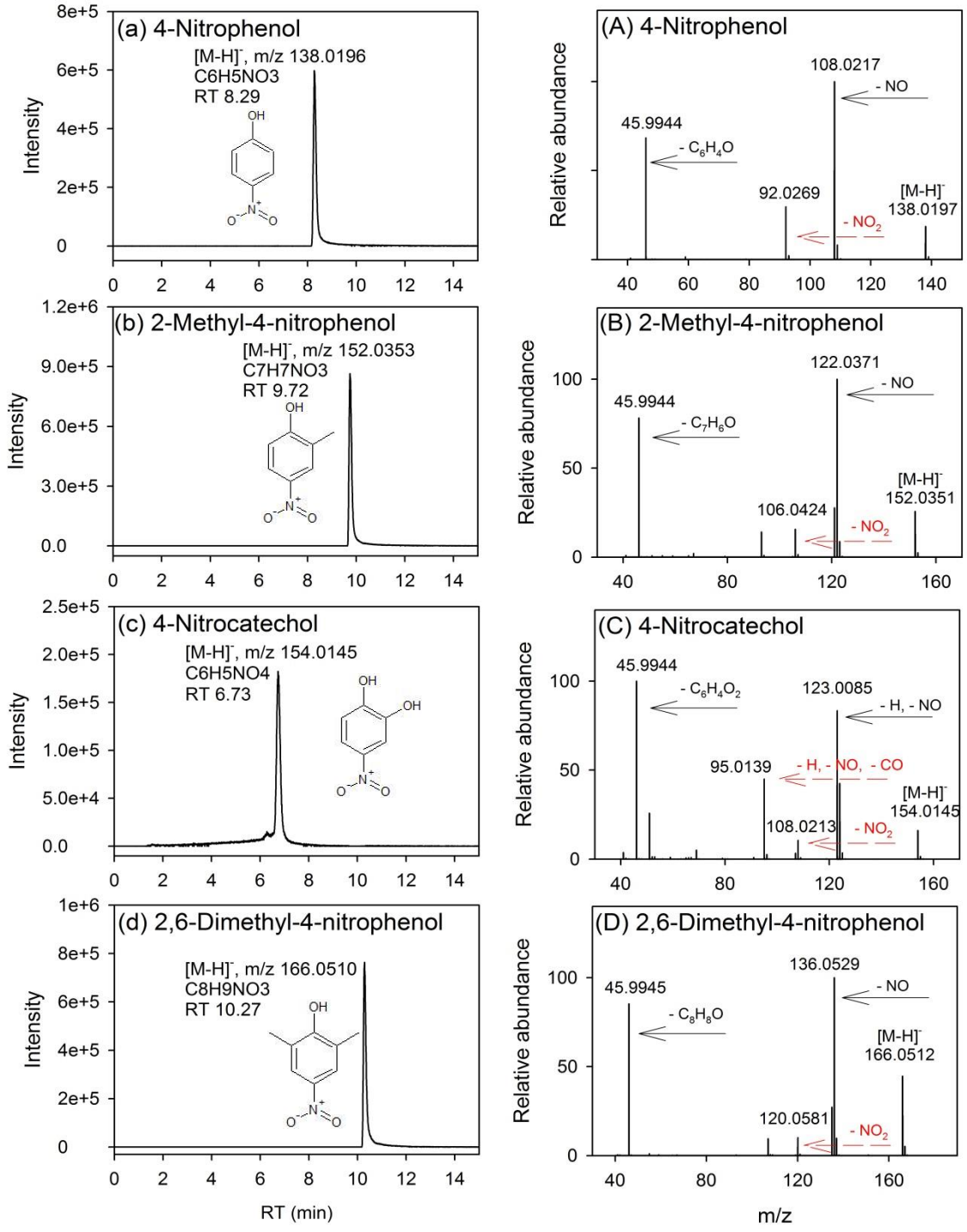


Figure S1. Extracted ion chromatograms (EICs) and Q-ToF MS/MS spectra for standard compounds, (a, A) 4-Nitrophenol, (b, B) 2-Methyl-4-nitrophenol, (c, C) 4-Nitrocatechol and (d, D) 2,6-Dimethyl-4-nitrophenol.

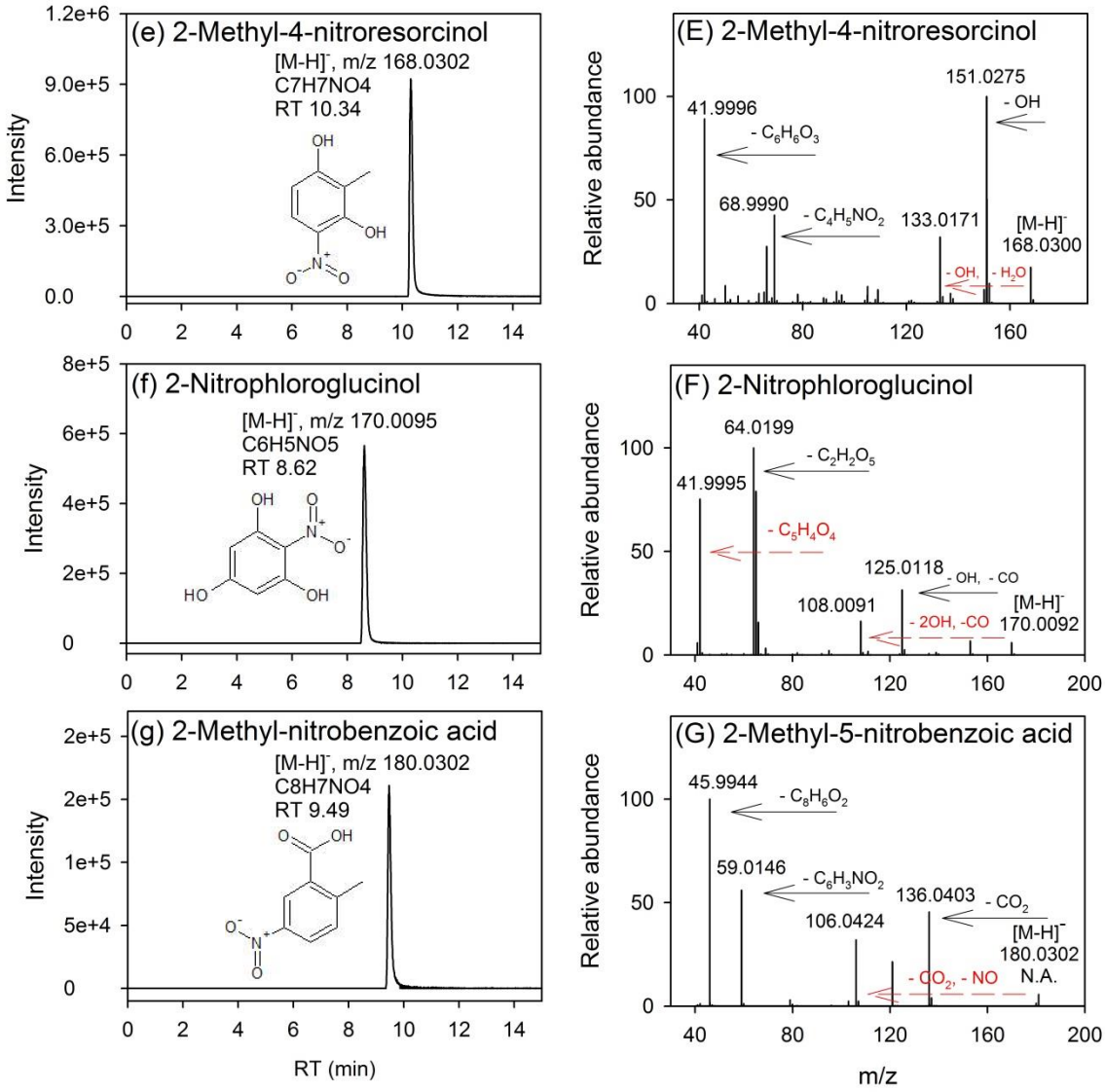


Figure S1. Continue, (e, E) 2-Methyl-4-nitroresorcinol, (f, F)2-Nitrophloroglucinol and (g, G) 2-Methyl-nitrobenzoic acid.

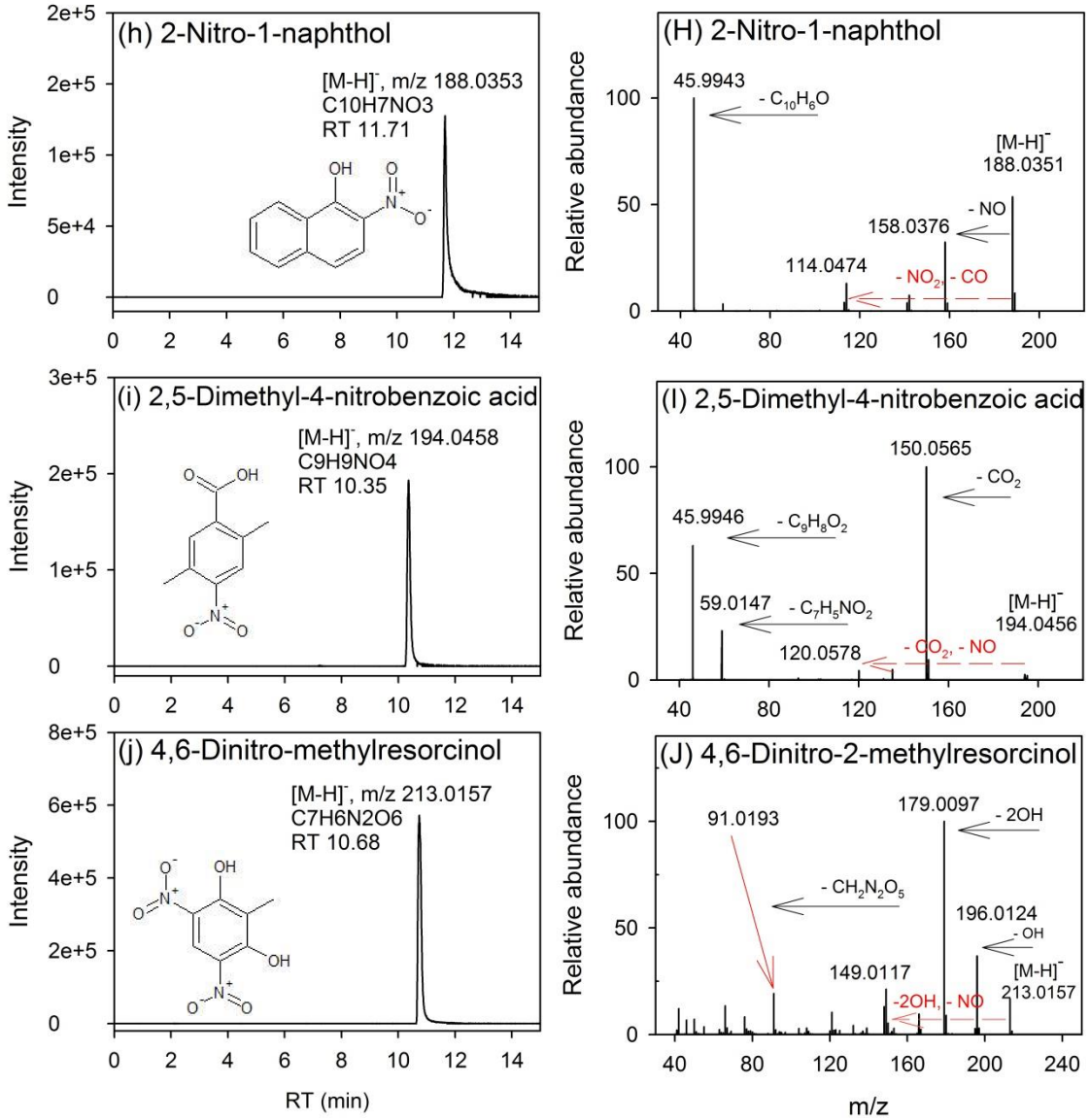


Figure S1. Continue, (h, H) 2-Nitro-1-naphthol, (i, I) 2, 5-Dimethyl-4-nitrobenzoic acid, and (j, J) 2,6-Dinitro-methylresorcinol.

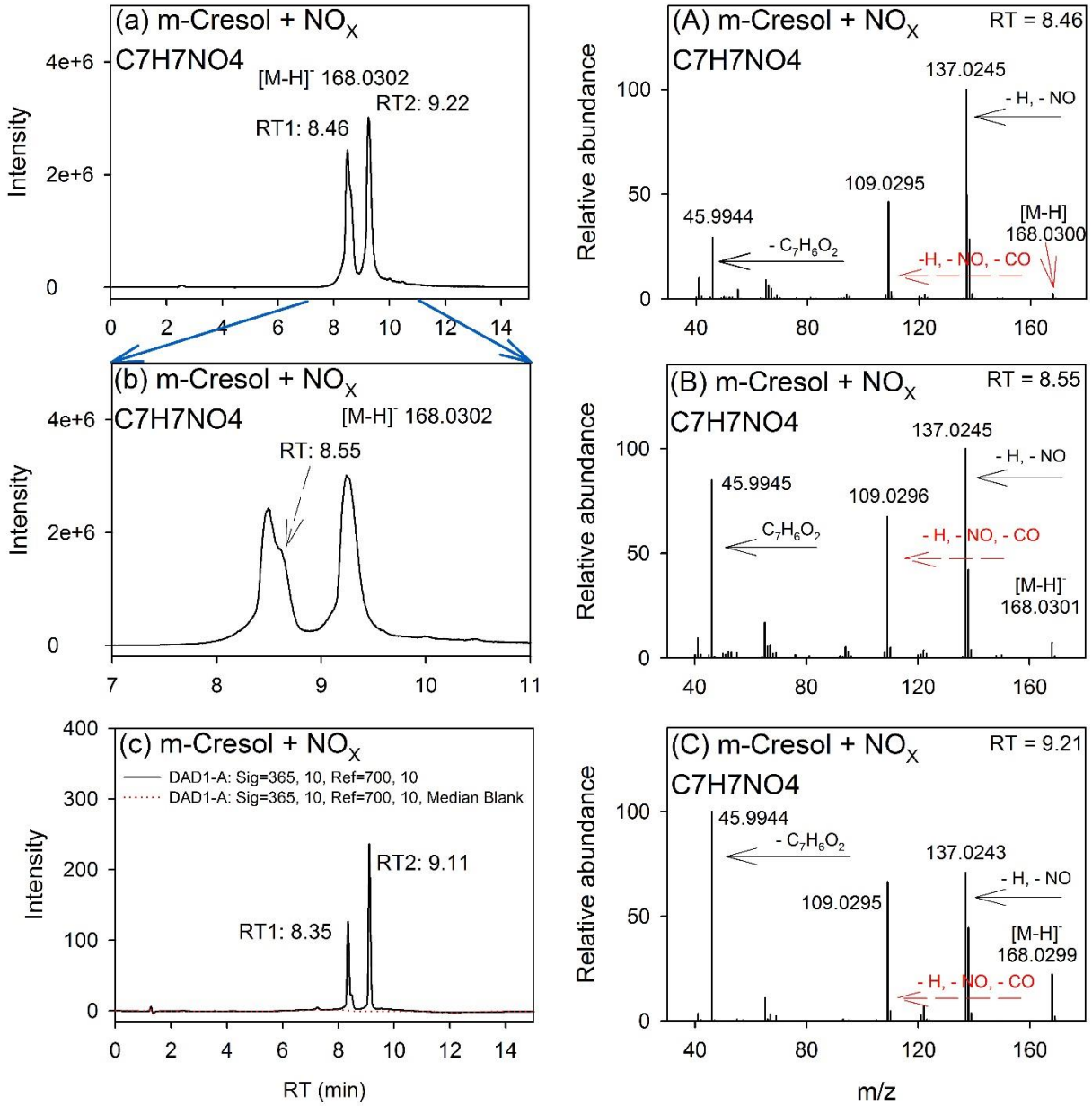


Figure S2. Extracted ion chromatograms (EICs) and Q-ToF MS/MS spectra of the $C_7H_7NO_4$ compounds (a, b, A-C) generated from *m*-cresol/NO_X reactions (Sample ER713 GF2), and (c) UV/Vis detector chromatogram (DAD signal) for this sample.

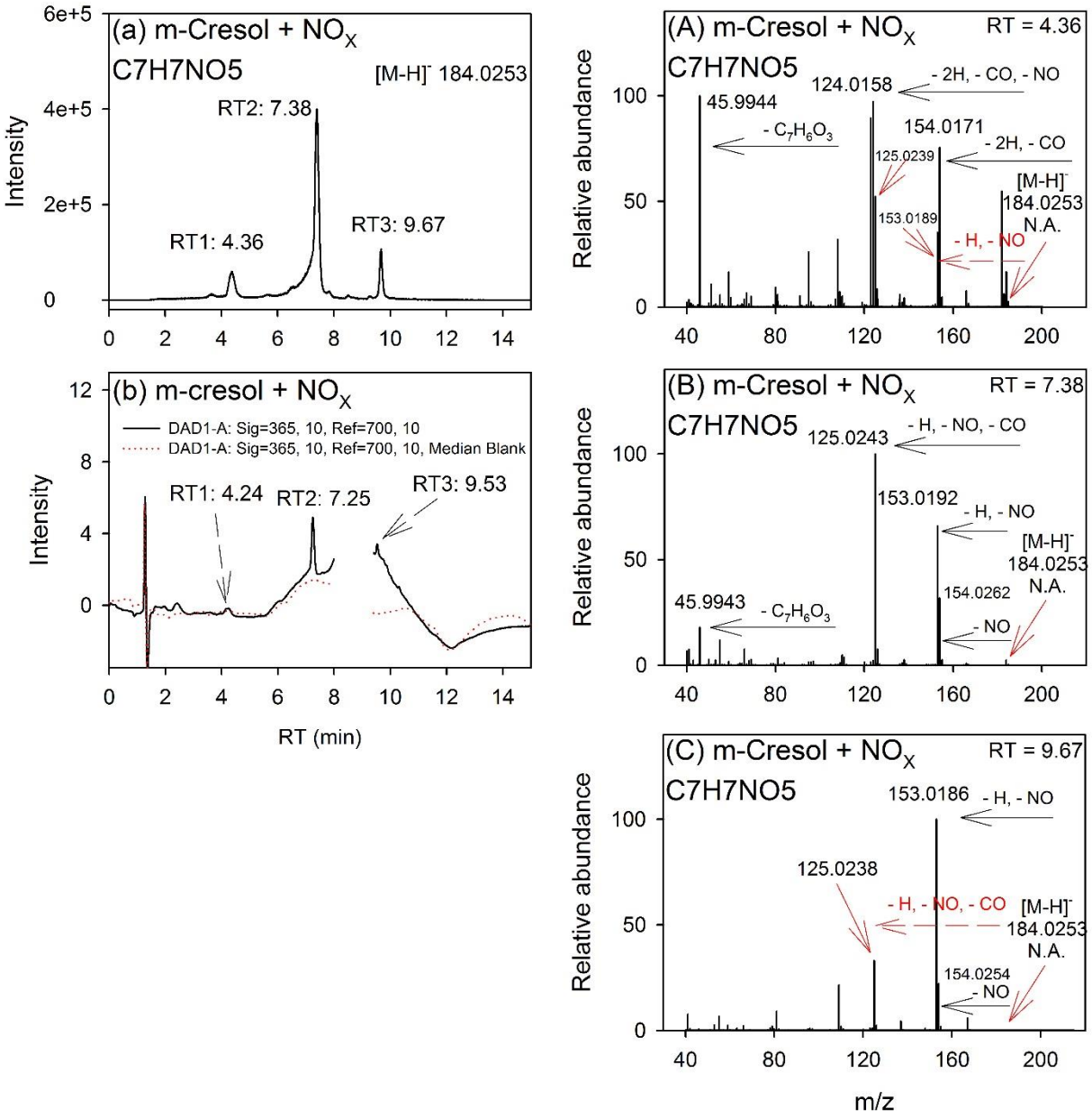


Figure S3. Extracted ion chromatogram (EIC) and Q-ToF MS/MS spectra of the $C_7H_7NO_5$ compounds (a, A-C) generated from *m*-cresol/NO_X reaction (Sample ER713 GF2), and (b) UV/Vis detector chromatogram (DAD signal) for this sample, omitting $C_7H_7NO_4$ signals.

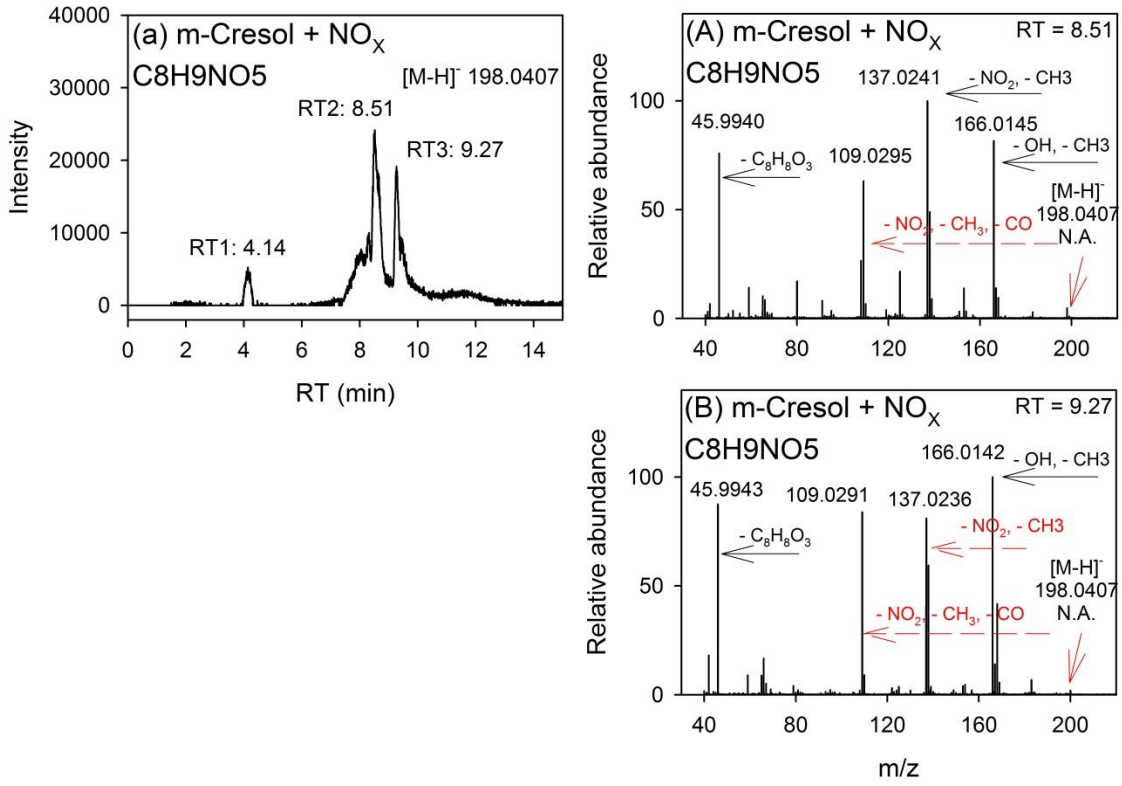


Figure S4. Extracted ion chromatogram (EIC) and Q-ToF MS/MS spectra of the $C_8H_9NO_5$ compounds (a, A, B) generated from *m*-cresol/NO_X reaction (Sample ER713 GF2). These compounds have low abundance and their absorbance at 365 nm could not be observed in UV/Vis detector chromatogram (DAD signal).

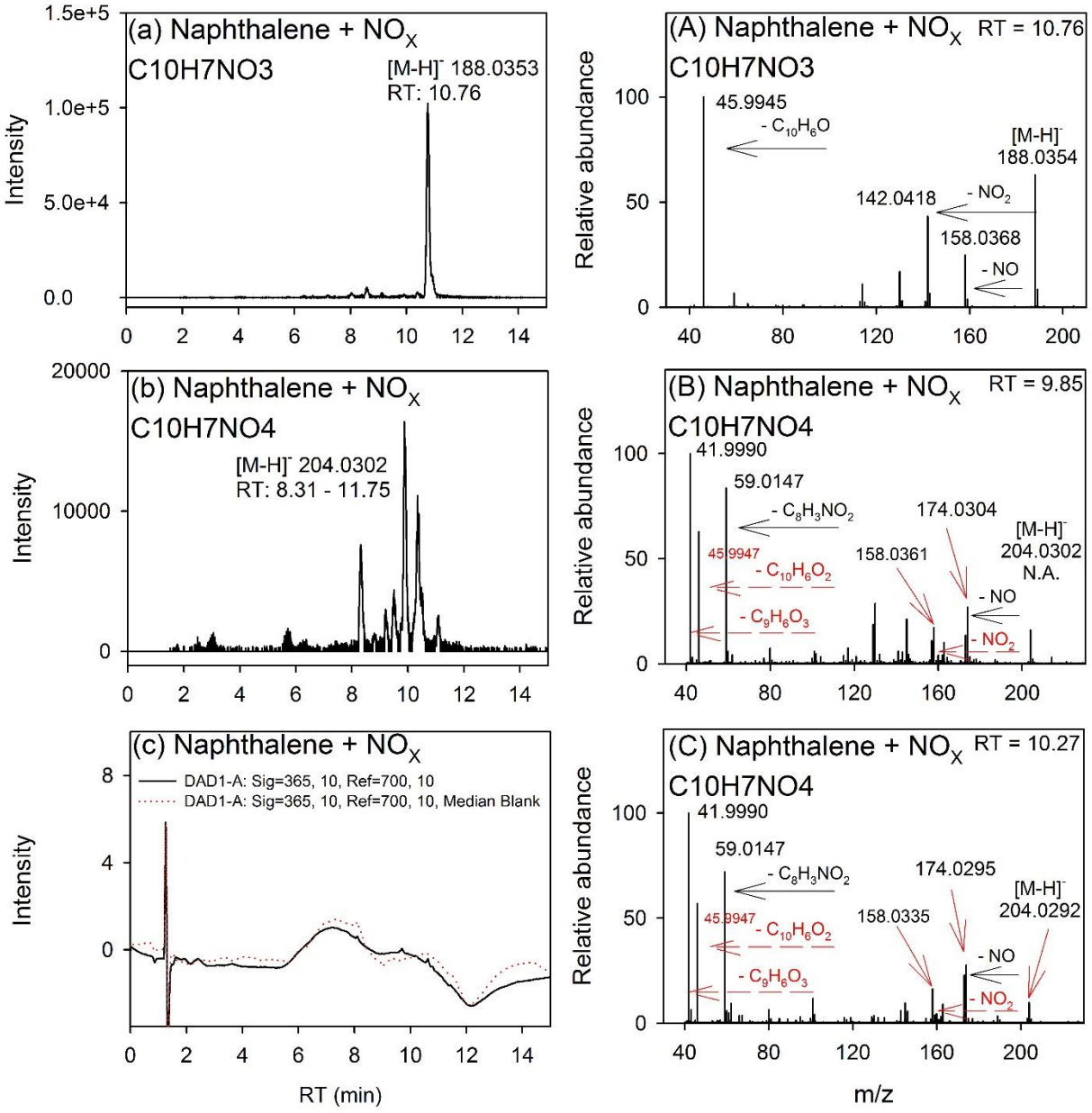


Figure S5. Extracted ion chromatograms (EICs) and Q-ToF MS/MS spectra of the $C_{10}H_7NO_3$ (a, A) and $C_{10}H_7NO_4$ (b, B, C) compounds generated from naphthalene/NO_X reaction (Sample 703 GF2), and (c) UV/Vis detector chromatogram (DAD signal) for this sample.

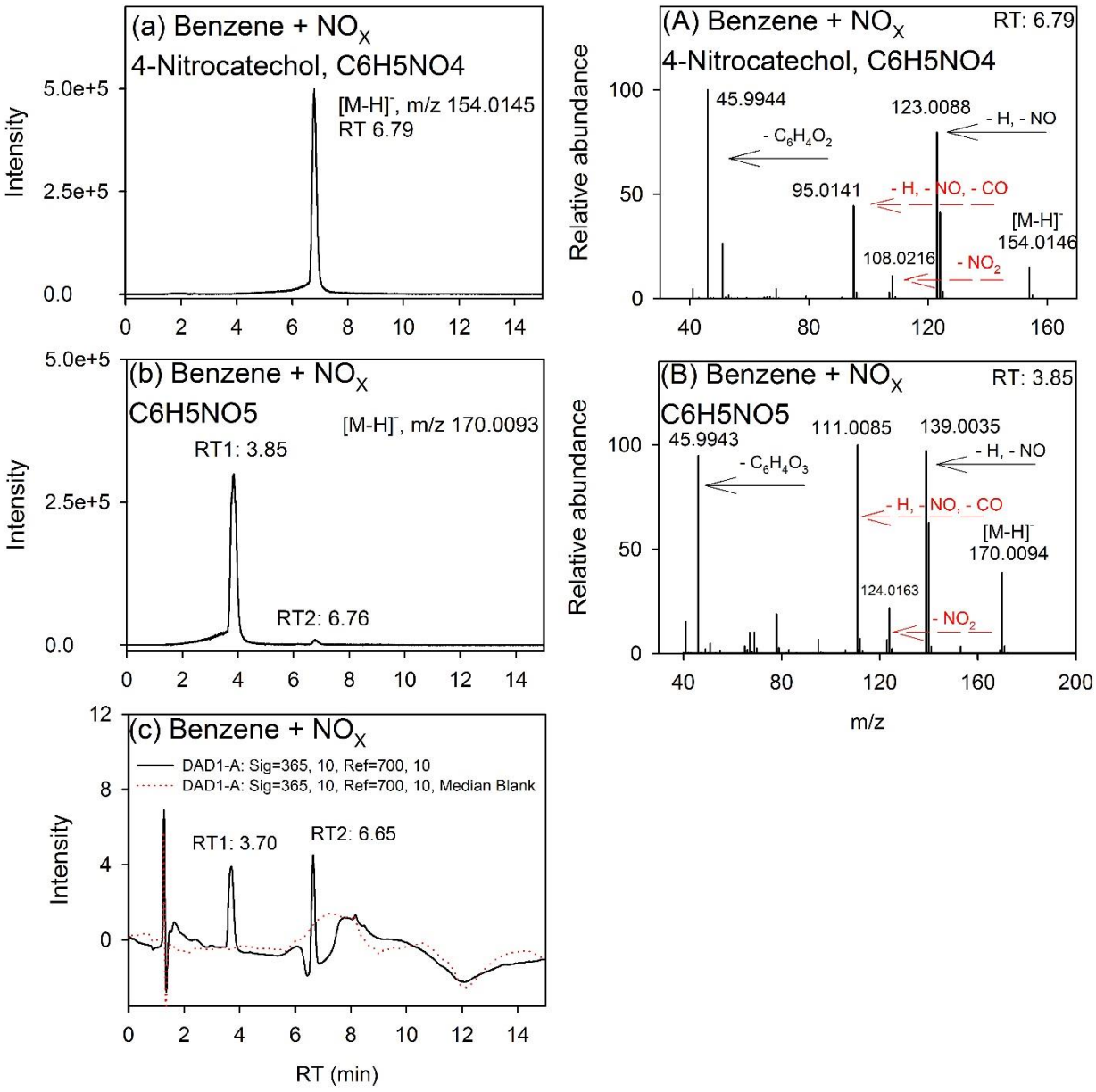


Figure S6. Extracted ion chromatograms (EICs) and Q-ToF MS/MS spectra of the $C_6H_5NO_4$ (a, A) and $C_6H_5NO_5$ (b, B) compounds generated from benzene/NO_X reaction (Sample ER542 GF4), and (c) UV/Vis detector chromatogram (DAD1) for this sample.

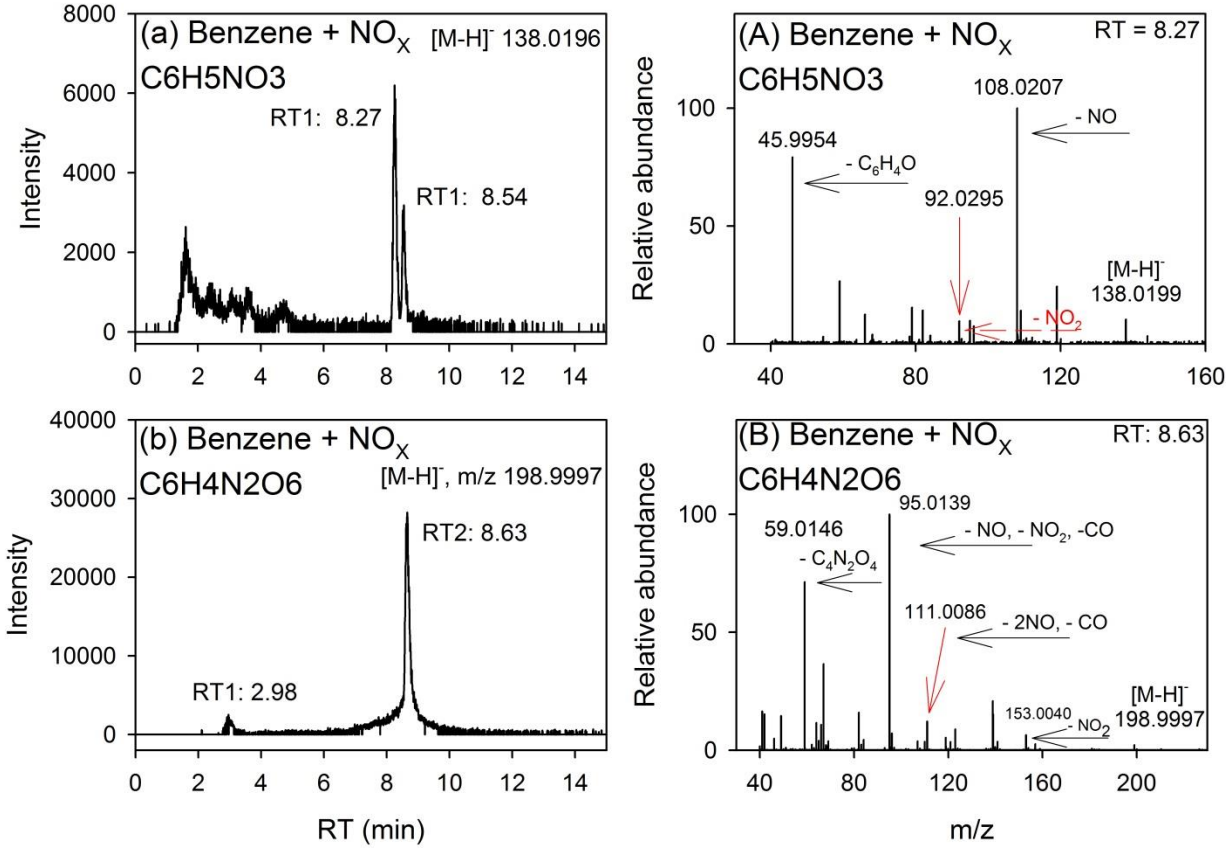


Figure S7. Extracted ion chromatograms (EICs) and Q-ToF MS/MS spectra of the $C_6H_5NO_3$ (a, A) and $C_6H_4N_2O_6$ (b, B) compounds generated from benzene/NO_X reaction (Sample ER542 GF4).

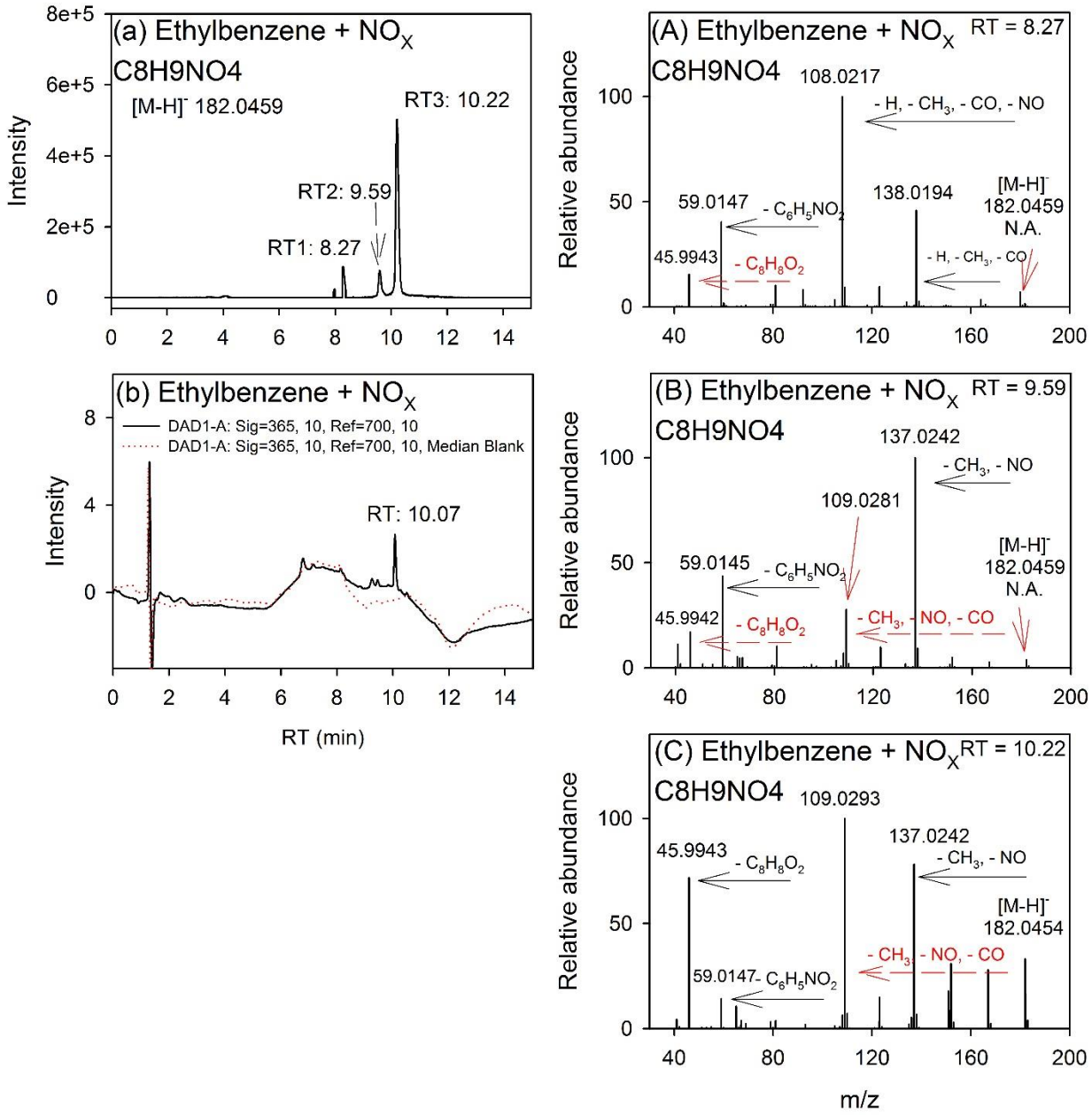


Figure S8. Extracted ion chromatogram (EIC) and Q-ToF MS/MS spectra of the $C_8H_9NO_4$ (a, A-C) compounds generated from ethylbenzene/NO_X reaction (Sample ER754 GF8), and (b) UV/Vis detector chromatogram (DAD signal) for this sample.

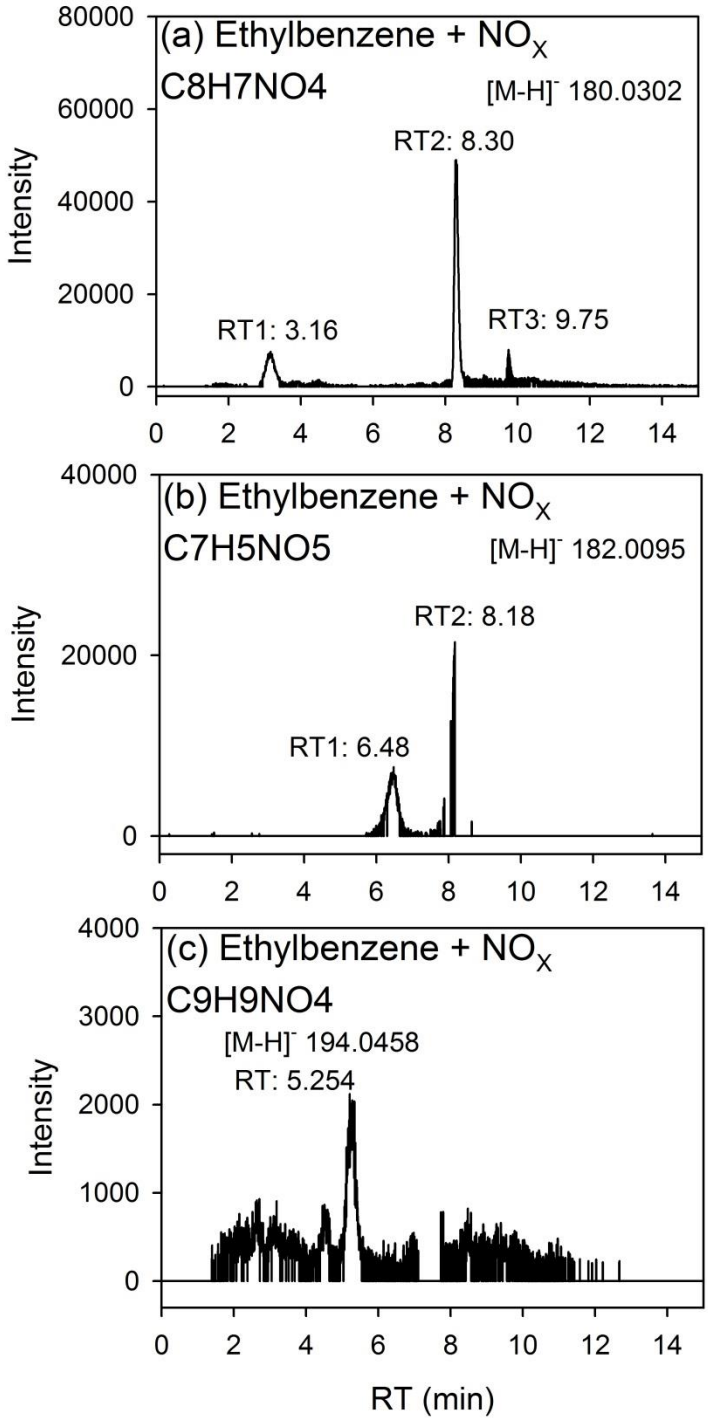


Figure S9. Extracted ion chromatograms (EICs) of (a) $C_8H_7NO_4$, (b) $C_7H_5NO_5$, and (c) $C_9H_9NO_4$ generated from ethylbenzene/NO_X reaction (Sample ER754 GF8).

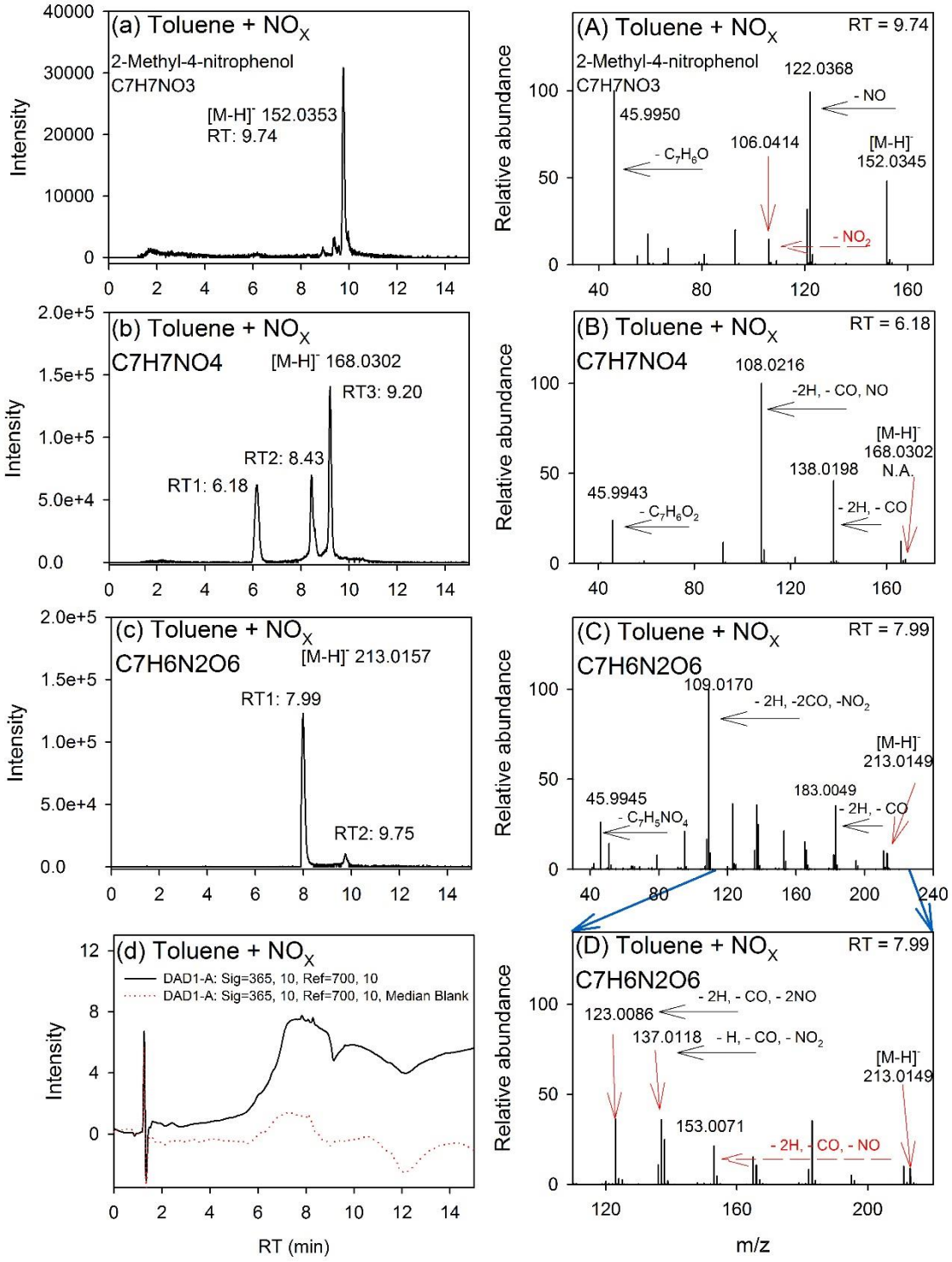


Figure S10. Extracted ion chromatograms (EICs) and Q-ToF MS/MS spectra of the $C_7H_7NO_3$ (a, A), $C_7H_7NO_4$ (b, B; MS/MS spectrum for compound eluting at 6.18 min), and $C_7H_6N_2O_6$ (c, C, D) compounds generated from toluene/NO_X reaction (Sample ER744 GF2), and (d) UV/Vis detector chromatogram (DAD sample) for this sample. Plot D is a magnification from m/z 110 to 220 of plot B.

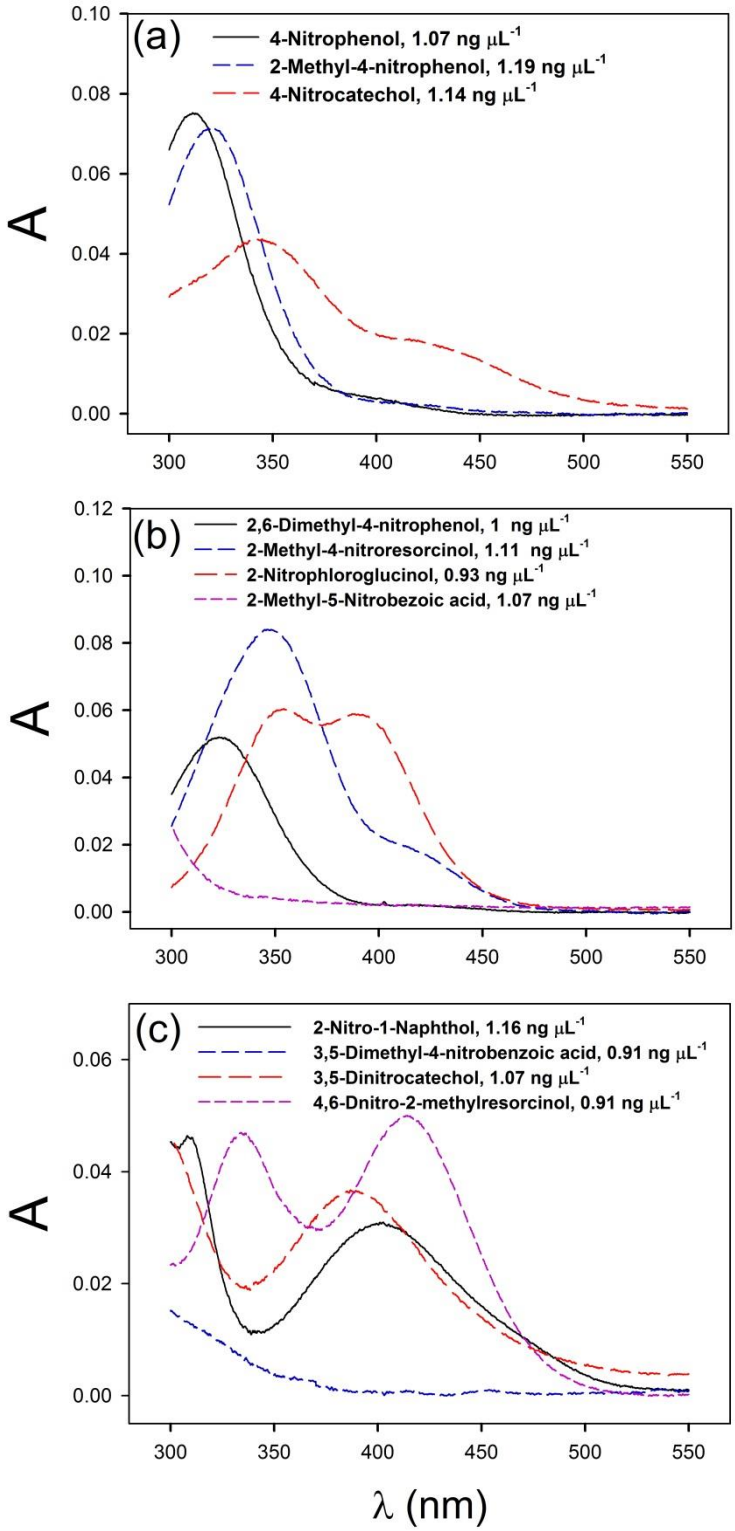


Figure S11. UV/Vis spectra ($A_{300\text{-}550} - A_{700}$) of standard compounds in methanol at around 1 ng μL^{-1}.

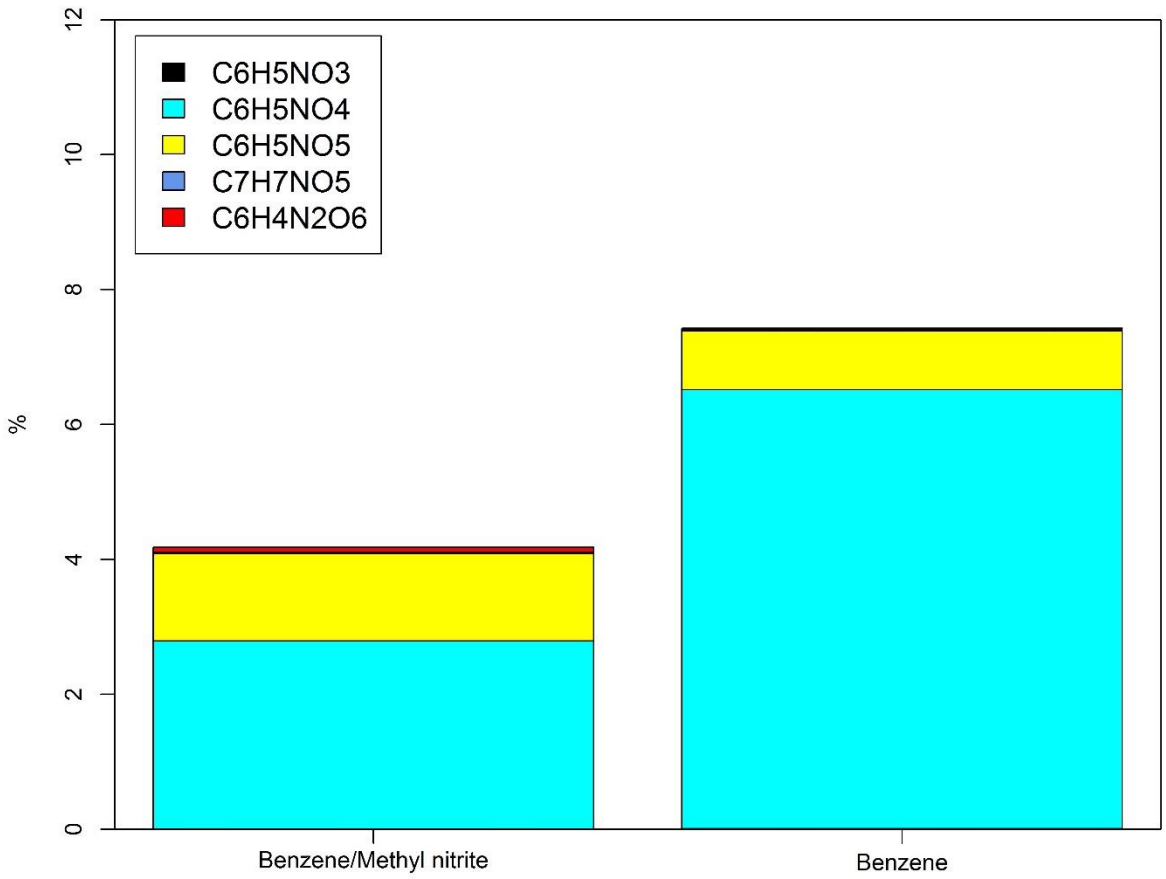


Figure S12. Average mass contributions (%) of nitro-aromatic compounds to total SOA generated from benzene/NO_X experiment under two different conditions. Four samples were collected from reactions with methyl nitrite, and the other four were collected from reactions without methyl nitrite.

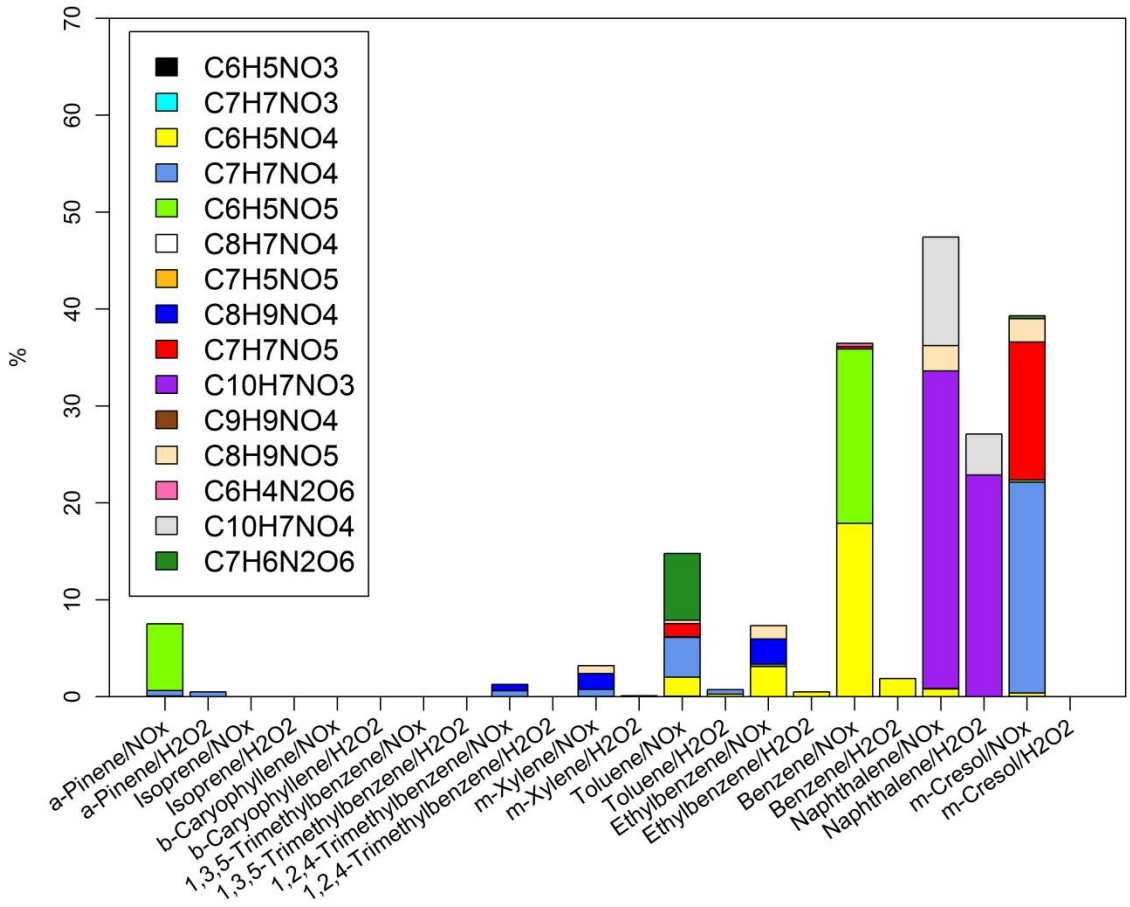


Figure S13. Average contributions (%) of nitro-aromatic compounds to Abs_{400} of total SOA generated in different chamber experiments.

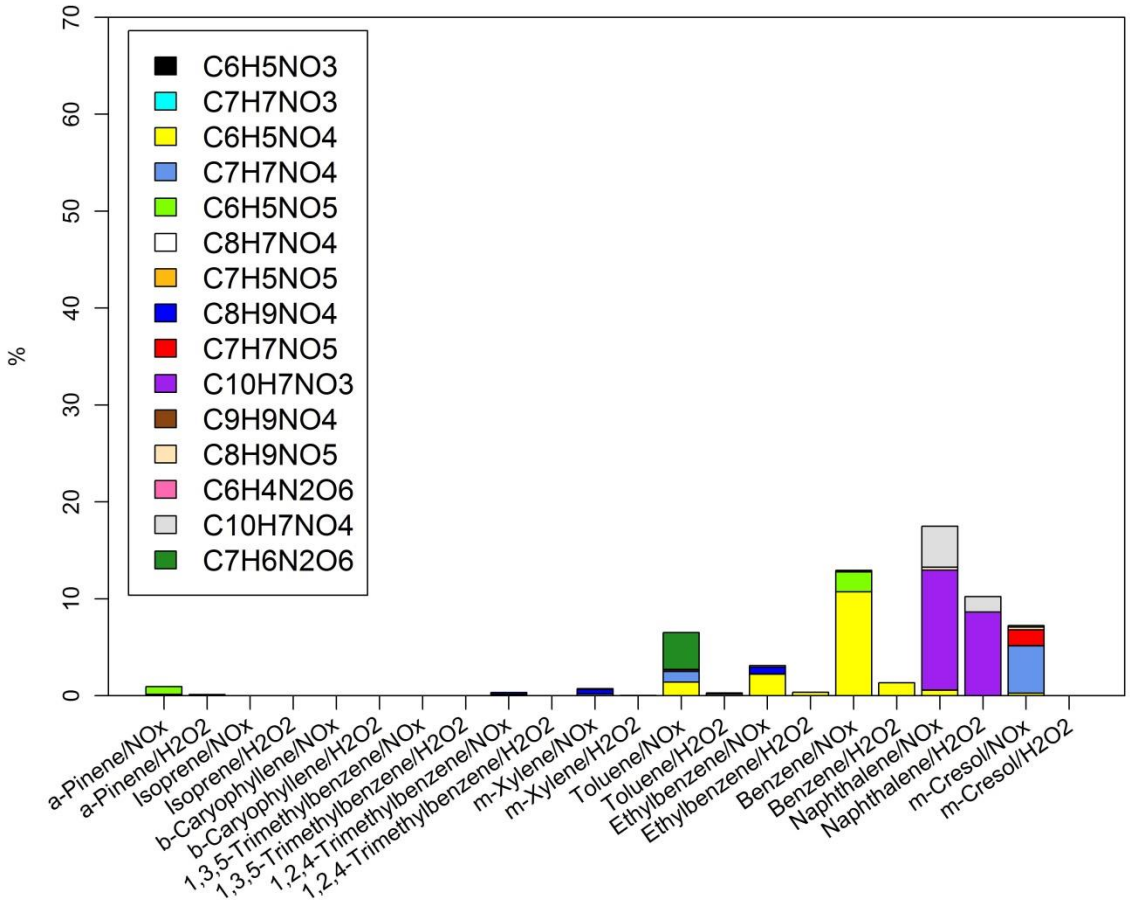


Figure S14. Average contributions (%) of nitro-aromatic compounds to Abs_{450} of total SOA generated in different chamber experiments.

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