Supplementary information for

"Composition and light absorption of nitroaromatic compounds in organic aerosols from laboratory biomass burning"

Mingjie Xie^{1,2,3,4,*}, Xi Chen⁴, Michael D. Hays⁴, Amara L. Holder⁴

¹Collaborative Innovation Center of Atmospheric Environment and Equipment Technology, Jiangsu Key Laboratory of Atmospheric Environment Monitoring and Pollution Control, School of Environmental Science and Engineering, Nanjing University of Information Science & Technology, 219 Ningliu Road, Nanjing 210044, China

²State Key Laboratory of Pollution Control and Resource Reuse, School of the Environment, Nanjing University, Nanjing, China

³Oak Ridge Institute for Science and Education (ORISE), Office of Research and Development, U.S. Environmental Protection Agency, 109 T.W. Alexander Drive, Research Triangle Pak, NC 27711, USA

⁴National Risk Management Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, 109 T.W. Alexander Drive, Research Triangle Pak, NC 27711, USA

*Correspondence to: Mingjie Xie E-mail: mingjie.xie@colorado.edu; mingjie.xie@nuist.edu.cn; Tel: +86-18851903788; Fax: +86-25-58731051; Mailing address: 219 Ningliu Road, Nanjing, Jiangsu, 210044, China

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1 Method

1.1 Light absorption measurement and data analysis

One filter punch (1.5 cm²) was extracted in 5 mL methanol (HPLC grade) ultrasonically for 15 min, and then filtered through a 30 mm diameter polytetrafluoroethylene (PTFE) filter with a 0.2 μ m pore size (National Scientific Company). The light absorption of methanol extracts was measured with a UV/Vis spectrometer over the wavelength (λ) range of 200 to 900 nm. To ensure data quality, the wavelength accuracy (\pm 0.3 nm) and repeatability (\pm 0.05 nm) were tracked every month with a NIST traceable Holmium Oxide standard. Solvent background was subtracted with a reference cuvette containing pure methanol. The extracted filter was air dried in a fume hood overnight, and the residual OC was measured with the Sunset thermaloptical analyzer. The extraction efficiency (η , %) of OC by methanol is calculated by:

$$\eta = \frac{\mathrm{OC_b} - \mathrm{OC_r}}{\mathrm{OC_b}} \times 100\% \tag{1}$$

where OC_b is the OC content of $PM_{2.5}$ filter before extraction and OC_r is the OC content in the air dried filter after extraction.

The light absorption coefficient of the methanol extracts (Abs_{λ}, Mm⁻¹) is calculated as:

$$Abs_{\lambda} = (A_{\lambda} - A_{700}) \times \frac{V_1}{V_a \times L} ln(10)$$
 (2)

where A_{700} is subtracted from A_{λ} to correct baseline drift, V_l (m³) is the solvent volume (5 mL) used for extraction, V_a (m³) is the air volume of the extracted filter area, L (0.01 m) is the optical path length, and ln (10) converts the absorption coefficient in units of m⁻¹ from log base-10 to natural log (Hecobian et al., 2010). The bulk mass absorption coefficient (MAC_{λ}, m² gC⁻¹) is calculated by:

$$MAC_{\lambda} = \frac{Abs_{\lambda}}{C_{OC}}$$
(3)

where C_{oc} is the mass concentration of extractable OC (OC_b – OC_r) for each filter sample (µg m⁻

³). The solution absorption Ångström exponent (Å_m) is determined from the slope of the linear regression of $log_{10}(Abs_{\lambda})$ vs. $log_{10}(\lambda)$ over the λ range of 300 to 550 nm. In the current work, Abs_{λ} and MAC_{λ} were focused at 365 nm and 550 nm, representing the BrC absorption at near UV and visible region, respectively.

1.2 Surrogate selection for analysis of nitroaromatic compounds (NACs)

Due to the lack of authentic standards, most of the NACs in BB samples were quantified using surrogates in this work. The surrogate compound with similar molecular weight and/or structure was selected for the mass quantification of each identified NAC.

Each identified NAC formula was assigned with an authentic or surrogate standard compound to estimate its contribution to Abs_{365} of extracted OM (Table S2). Except for $C_8H_7NO_4$ and $C_9H_9NO_4$, the standard compounds used for the estimation of NACs absorption and NACs mass quantification are the same (Table S2). The light absorption of organic compounds is strongly associated with the degree of conjugation (Chen and Bond, 2010;Laskin et al., 2015). In this work, the structures of $C_8H_7NO_4$ and $C_9H_9NO_4$ in BB emission samples are different from 2-methyl-5-nitrobenzoic acid ($C_8H_7NO_4$) and 2,5-dimethyl-4-nitrobenzoic acid ($C_9H_9NO_4$), respectively, since the loss of CO_2 was not observed in their MS/MS spectra (Fig. S2f,g,l, and m). Moreover, each of these two NACs is expected to have at least three phenoxyl groups with much higher degrees of conjugation than nitrobenzoic acids (Table S2). As such, the 2-nitrophloroglucinol with three phenolic groups was used to estimate the absorption of $C_8H_7NO_4$ and $C_9H_9NO_4$ in BB emission samples.

Date	Burn case	Sample phase	Sample volume (m ³)	OC (mg m ⁻³)	EC (mg m ⁻³)	EC/OC	Extraction efficiency (%)	MAC ₃₆₅ (m ² gC ⁻¹)	MAC ₅₅₀ (m ² gC ⁻¹)	Å _{abs}
FL forest ^a										
11/16/2012	Burn 1	Whole	0.45	1.90	0.22	0.12	98.8	1.03	0.037	7.79
11/16/2012	Burn 2	Whole	0.13	3.82	0.58	0.15	99.1	1.06	0.041	7.80
11/16/2012	Burn 3	Whole	0.14	1.56	0.91	0.58	98.6	1.30	0.11	6.00
11/16/2012	Burn 4	Whole	0.26	14.1	0.38	0.027	98.6	0.92	0.030	8.01
11/16/2012	Burn 5	Whole	0.26	2.76	0.44	0.16	95.6	1.16	0.056	7.33
11/16/2012	Burn 6	Whole	0.19	6.14	0.81	0.13	96.1	1.01	0.043	7.34
11/16/2012	Burn 7	Whole	0.21	4.96	1.09	0.22	97.0	1.04	0.045	7.58
11/16/2012	Burn 8	Whole	0.21	2.77	0.64	0.23	95.9	1.32	0.059	7.15
11/16/2012	Burn 9	Whole	0.23	3.46	0.90	0.26	93.6	1.32	0.059	7.22
Average Temp	. 10 °C, Avera	age Humidity 83%								
				NC fo	rest 1					
4/16/2016	Burn 1	Flaming	0.0038	86.1	2.79	0.032	97.2	1.18	0.077	6.47
		Smoldering	0.024	17.9	0.13	0.0072	97.6	0.96	0.043	7.17
	Burn 2	Flaming	0.039	21.0	0.76	0.036	97.9	1.63	0.17	5.42
		Smoldering	0.063	4.32	0.052	0.012	98.0	1.12	0.070	6.23
	Burn 3	Flaming	0.032	17.4	1.02	0.059	97.9	1.60	0.20	5.15
		Smoldering	0.14	3.63	0.037	0.010	98.0	0.91	0.047	7.10
Average Temp	. 12 °C, Avera	age Humidity 49%								
				NC fo	rest 2					
7/14/2016	Burn 1	Flaming	0.025	44.7	1.60	0.036	99.0	3.97	0.17	7.40
		Smoldering	0.073	15.1	0.15	0.010	99.1	3.75	0.15	7.79
	Burn 2	Flaming	0.037	34.2	2.13	0.062	99.7	4.25	0.18	7.44
		Smoldering	0.057	12.1	0.11	0.0091	99.3	3.15	0.081	8.22
	Burn 3	Flaming	0.036	39.4	1.84	0.047	99.7	4.14	0.17	7.41
		Smoldering	0.11	11.8	0.080	0.0067	99.3	3.19	0.13	7.74
	Burn 4	Flaming	0.039	35.1	1.86	0.053	99.5	3.92	0.18	7.28
		Smoldering	0.12	11.0	0.046	0.0042	99.2	2.92	0.10	8.03
Average Temp	. 29 °C, Avera	age Humidity 70%								

 Table S1. Sample information for the laboratory simulations in open burn test facility (OBTF).

^a Data were obtained from Xie et al. (2017b)

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	138.0198		4-Nitrophenol (C ₆ H₅NO ₃)	4-Nitrophenol (C ₆ H₅NO ₃)
C ₆ H ₅ NO ₄	154.0145	154.0143	OH O'N [*] OH	4-Nitrocatechol (C ₆ H₅NO ₄)	4-Nitrocatechol (C ₆ H ₅ NO ₄)
C7H7NO4 (Iso1)	168.0302	168.0295	HO CH3	2-Methyl-4-nitroresorcinol	2-Methyl-4-nitroresorcinol
C7H7NO4 (Iso2)	168.0302	168.0291	OF OH OF OH OH OH	2-Methyl-4-nitroresorcinol	2-Methyl-4-nitroresorcinol
$C_6H_5NO_5$	170.0095	170.0087	HO O ⁺ OH	2-Nitrophloroglucinol (C ₆ H ₅ NO ₅)	2-Nitrophloroglucinol (C ₆ H ₅ NO ₅)
$C_8H_7NO_4$ (Iso1)	180.0302	180.0305	HO HO H ₃ C ^{-O}	2-Methyl-5-nitrobenzoic acid	2-Nitrophloroglucinol (C ₆ H ₅ NO ₅)
C ₈ H7NO₄ (Iso2)	180.0302	180.0290	HO CH3	2-Methyl-5-nitrobenzoic acid (C ₈ H ₇ NO ₄)	2-Nitrophloroglucinol (C ₆ H ₅ NO ₅)

Table S2. Identified nitroaromatic com	pounds by HPLC/ESI-C)-ToFMS from laboratory	v biomass burning i	in this study.
Table 52. Identified inter our officie com			y bromass burning i	III UIIIS Study

^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 ₈ H ₉ NO₄ (Iso1)	182.0459	182.0467	H ₃ C H ₃ OH H ₃ C N [*] :0	2-Methyl-4-nitroresorcinol $(C_7H_7NO_4)$	2-Methyl-4-nitroresorcinol (С ₇ H ₇ NO ₄)
C ₈ H ₉ NO₄ (Iso2)	182.0459	182.0452	CH ₃ OH O ^N OH	2-Methyl-4-nitroresorcinol (C ₇ H ₇ NO ₄)	2-Methyl-4-nitroresorcinol (C ₇ H ₇ NO ₄)
C ₇ H ₇ NO ₅	184.0253	184.0259	CH ₃ OH OH OH	PH PL	$\overset{OH}{\underset{HO}{}}\overset{OH}{\underset{OH}{}}\overset{OH}{\underset{OH}{}}$ 2-Nitrophloroglucinol (C ₆ H ₅ NO ₅)
$C_{10}H_7NO_3$	188.0353	188.0356	OH OH	2-Nitro-1-naphthol (C ₁₀ H ₇ NO ₃)	2-Nitro-1-naphthol (C ₁₀ H ₇ NO ₃)
C₀H₀NO₄ (Iso1)	194.0458	194.0461	H ₃ C O H ₃ C	2,5-Dimethyl-4-nitrobenzoic acid (C₀H₀NO₄)	$2-Nitrophloroglucinol (C_6H_5NO_5)$
C ₉ H ₉ NO ₄ (Iso2)	194.0458	194.0461	HO HO HO HO HO	2,5-Dimethyl-4-nitrobenzoic acid	$2-Nitrophloroglucinol(C_6H_5NO_5)$
C ₈ H ₉ NO₅	198.0407	198.0407	H ₃ C 0 N ⁺² O	2-Nitrophloroglucinol (C ₆ H ₅ NO 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 ₁₀ H ₁₁ NO ₄ (Iso1)	208.0615	208.0621	H ₃ CH H ₃ C	2-Nitrophloroglucinol (C ₆ H ₅ NO ₅)	2-Nitrophloroglucinol (C ₆ H ₅ NO ₅)
C ₁₀ H ₁₁ NO ₄ (Iso2)	208.0615	208.0607	Ho Ho Ho Ho	2-Nitrophloroglucinol $(C_6H_5NO_5)$	2-Nitrophloroglucinol $(C_6H_5NO_5)$
C ₁₀ H ₁₁ NO ₄ (Iso3)	208.0615	208.0616	O OH H ₃ C OH H ₃ C CH ₃	2-Nitrophloroglucinol $(C_6H_5NO_5)$	2-Nitrophloroglucinol ($C_6H_5NO_5$)
$C_{10}H_{11}NO_5$	224.0564	224.0565	H ₃ C O CH ₃	2-Nitrophloroglucinol $(C_6H_5NO_5)$	2-Nitrophloroglucinol $(C_6H_5NO_5)$
$C_{11}H_{13}NO_5$	238.0721	238.0722	H_3C CH_3 OH H_3C CH_3 CH_3	$2-Nitrophloroglucinol(C_6H_5NO_5)$	2-Nitrophloroglucinol ($C_6H_5NO_5$)
C ₁₁ H ₁₃ NO ₆	254.0670	254.0670	H_3C OH H_3C H_3C	2-Nitrophloroglucinol ($C_6H_5NO_5$)	$2-Nitrophloroglucinol(C_6H_5NO_5)$

Standard compounds ^a	Formula	<i>m/z</i> , [M-H] ⁻	Recovery ($N^{b} = 4, \%$)	Detection Limit (pg)
4-Nitrophenol	$C_6H_5NO_3$	138.0196	$97.7 \pm 0.92^{\circ}$	4.25
4-Nitrocatechol	$C_6H_5NO_4$	154.0145	75.1 ± 0.48	4.79
2-Methyl-4-nitroresocinol	C ₇ H ₇ NO 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 ₈ H ₇ NO 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

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

^a Data were obtained from Xie et al. (2017a) ; ^b Number of repetition; ^c mean ± standard deviation.

Suggested	m/z	EL Eorest	NC Fo	orest 1	NC Fo	NC Forest 2		
formula	[M-H] ⁻	(<i>N</i> = 9)	Flaming (N =3)	Smoldering (N =3)	Flaming (N =4)	Smoldering (N =4)		
$C_6H_5NO_3$	138.0196	0.0011±0.0005 (0.0004 – 0.0016)	/ ^a	/	/	/		
$C_6H_5NO_4$	154.0145	0.029 ± 0.011 (0.0069 - 0.043)	0.037 ± 0.011 (0.025 – 0.046)	0.024 ± 0.0098 (0.015 - 0.035)	0.033 ± 0.011 (0.018 - 0.044)	0.010 ± 0.0027 (0.0060 - 0.012)		
C ₇ H ₇ NO ₄	168.0301	0.014 ± 0.0064 (0.0037 - 0.023)	0.017 ± 0.0059 (0.011 – 0.022)	0.0087 ± 0.0030 (0.0054-0.011)	0.016 ± 0.0052 (0.0081 - 0.020)	0.0043 ± 0.0010 (0.0029 - 0.0052)		
$C_6H_5NO_5$	170.0093	0.0067 ± 0.0045 (0.0012 - 0.012)	0.011 ± 0.0069 (0.0042 - 0.018)	/	0.016 ± 0.0042 (0.011 - 0.020)	0.0009 ± 0.0005 (0.0003 - 0.0013)		
C ₈ H ₇ NO ₄	180.0302	0.013 ± 0.0056 (0.0035 - 0.018)	0.012 ± 0.0055 (0.0074 - 0.018)	/	0.014 ± 0.0035 (0.0089 - 0.017)	/		
$C_8H_9NO_4$	182.0459	0.0082 ± 0.0052 (0.0008 - 0.015)	0.012 ± 0.0057 (0.0059 - 0.017)	0.0047 ± 0.0018 (0.0028 - 0.0064)	0.0086 ± 0.0037 (0.0035 - 0.012)	0.0021±0.0008 (0.0012 - 0.0029)		
C ₇ H ₇ NO ₅	184.0253	0.0036 ± 0.0019 (0.0011 - 0.0056)	0.0075 ± 0.0044 (0.0028 - 0.012)	0.0017 ± 0.0012 (0.0004 - 0.0028)	0.0063 ± 0.0024 (0.0035 - 0.0086)	/		
$C_{10}H_7NO_3$	188.0353	0.0067 ± 0.0024 (0.0041 - 0.0089)	0.0033 ± 0.0007 (0.0025 - 0.0037)	/	0.0063 ± 0.0001 (0.0062 - 0.0064)	/		
$C_9H_9NO_4$	194.0458	0.023 ± 0.012 (0.0057 - 0.043)	0.049 ± 0.016 (0.032 - 0.063)	0.0052 ± 0.0033 (0.0028 - 0.0089)	0.035 ± 0.0072 (0.024 - 0.040)	$0.0047 \pm 0.0013^{\circ}$ (0.0035 - 0.0060)		
$C_8H_9NO_5$	198.0407	0.0072 ± 0.0034 (0.0015 - 0.011)	0.0056 ± 0.0027 ($0.0025 - 0.0073$)	0.0025 ± 0.0016 (0.0010 - 0.0042)	0.0051 ± 0.0017 (0.0030 - 0.0073)	/		
$C_{10}H_{11}NO_4$	208.0615	0.0069 ± 0.0030 (0.0021 - 0.011)	0.012 ± 0.0078 (0.0036 - 0.019)	0.0044 ± 0.0023 (0.0023 - 0.0068)	0.014 ± 0.0036 (0.0093 - 0.018)	0.0019 ± 0.0008 (0.0009 - 0.0027)		
$C_{10}H_{11}NO_5$	224.0564	0.0057 ± 0.029 (0.0025 - 0.010)	0.0041 ± 0.0005 [▷] (0.0036 - 0.0046)	/	0.0032 ± 0.0009 (0.0021 - 0.0038)	$\begin{array}{c} 0.0007 \pm 0.0004 \\ (0.0003 - 0.0012) \end{array}$		
$C_{11}H_{13}NO_5$	238.0721	0.012 ± 0.0060 (0.0043 - 0.022)	0.0062 ± 0.0030 (0.0032 - 0.0093)	0.0029 ± 0.0025 (0.0014 - 0.0058)	0.0035 ± 0.0013 (0.0016 - 0.0045)	0.0016 ± 0.0003 (0.0014 - 0.0019)		
$C_{11}H_{13}NO_6$	254.067	0.0005 ± 0.0003 (0.0002 - 0.0010)	/	/	$\begin{array}{c} 0.0003 \pm 0.0000 \\ (0.0002 - 0.0003) \end{array}$	/		
Subtotal (tNAC _{OM} %)		0.13 ± 0.059 (0.037 – 0.21)	0.18 ± 0.067 (0.10 - 0.23)	0.055 ± 0.026 (0.032 - 0.082)	0.16 ± 0.045 (0.091 – 0.20)	0.023 ± 0.0089 (0.013 – 0.031)		

Table S4. Average and ranges of mass contribution (%) of identified nitroaromatic compounds to organic matter in PM_{2.5} from laboratory biomass burning.

^a Not detected; ^b detected in two samples, the value represents average $\pm |x1-x2|/2$.

NAC	m/z	
formula	[M-H] ⁻	WAC 365, OM
$C_6H_5NO_3$	138.0196	2.44
$C_6H_5NO_4$	154.0145	7.02
C ₇ H ₇ NO ₄	168.0302	12.9
$C_6H_5NO_5$	170.0095	14.0
C ₈ H ₇ NO ₄	180.0302	14.0
C ₈ H ₉ NO ₄	182.0459	12.9
$C_7H_7NO_5$	184.0253	14.0
$C_{10}H_7NO_3$	188.0353	3.75
C ₉ H ₉ NO₄	194.0458	14.0
C ₈ H ₉ NO ₅	198.0407	14.0
$C_{10}H_{11}NO_4$	208.0615	14.0
$C_{10}H_{11}NO_5$	224.0564	14.0
$C_{11}H_{13}NO_5$	238.0721	14.0
$C_{11}H_{13}NO_{6}$	254.0670	14.0

Table S5. $MAC_{365, NAC}$ (m² g⁻¹) values for identified NAC formulas.

^a Obtained from Xie et al. (2017a)

Suggested	m/z	FL Forest	NC Fo	orest 1	NC Fo	NC Forest 2		
formula	[M-H] ⁻	(N = 9)	Flaming (N =3)	Smoldering (N =3)	Flaming (N =4)	Smoldering (N =4)		
$C_6H_5NO_3$	138.0196	0.0042 ± 0.0016 (0.0018 - 0.0066)	/ ^a	/	/	/		
$C_6H_5NO_4$	154.0145	0.31 ± 0.11 (0.091 – 0.42)	0.30 ± 0.045 (0.26 - 0.35)	0.29 ± 0.095 (0.19 - 0.37)	0.098 ± 0.034 (0.055 - 0.13)	0.037 ± 0.0080 (0.025 - 0.042)		
C ₇ H ₇ NO ₄	168.0301	0.27 ± 0.12 (0.090 - 0.40)	0.26 ± 0.050 (0.21 - 0.31)	0.19 ± 0.058 (0.13– 0.23)	0.084 ± 0.029 (0.045 - 0.11)	0.029 ± 0.0051 (0.022 - 0.034)		
$C_6H_5NO_5$	170.0093	0.14 ± 0.094 (0.022 - 0.27)	0.17 ± 0.091 (0.088 – 0.27)	/	0.092 ± 0.025 (0.065 - 0.11)	0.0067 ± 0.0034 (0.0028 - 0.0091)		
$C_8H_7NO_4$	180.0302	0.28 ± 0.11 (0.093 – 0.37)	0.20 ± 0.066 (0.15 - 0.27)	/	0.079 ± 0.020 (0.54 - 0.10)	/		
$C_8H_9NO_4$	182.0459	0.16 ± 0.097 (0.013 - 0.27)	0.18 ± 0.062 (0.11 - 0.24)	0.11 ± 0.034 (0.067 – 0.13)	0.047 ± 0.020 (0.020 - 0.068)	0.014 ± 0.0055 (0.0091 – 0.020)		
$C_7H_7NO_5$	184.0253	0.077 ± 0.040 (0.029 - 0.13)	0.12 ± 0.057 (0.058 - 0.17)	0.040 ± 0.026 (0.011 – 0.062)	0.037 ± 0.015 (0.021 - 0.053)	/		
$C_{10}H_7NO_3$	188.0353	0.040 ± 0.013 (0.027 - 0.056)	0.015 ± 0.0047 (0.010 - 0.019)	/	0.0098 ± 0.0004 (0.0094 - 0.010)	/		
$C_9H_9NO_4$	194.0458	0.47 ± 0.21 (0.15 – 0.82)	0.79 ± 0.14 (0.67 - 0.94)	0.12 ± 0.063 (0.072 - 0.19)	0.21 ± 0.041 (0.15 – 0.24)	$0.032 \pm 0.062^{\circ}$ (0.026 - 0.038)		
$C_8H_9NO_5$	198.0407	0.15 ± 0.066 (0.039 - 0.24)	0.088 ± 0.032 (0.051 - 0.11)	0.058 ± 0.032 (0.026 - 0.090)	0.030 ± 0.011 (0.018 – 0.045)	/		
$C_{10}H_{11}NO_4$	208.0615	0.15 ± 0.053 (0.055 – 0.21)	0.19 ± 0.10 (0.074 – 0.28)	0.10 ± 0.045 (0.058 – 0.15)	0.083 ± 0.022 (0.056 - 0.11)	0.014 ± 0.0048 (0.0072 - 0.018)		
$C_{10}H_{11}NO_5$	224.0564	0.12 ± 0.049 (0.067 - 0.19)	$0.062 \pm 0.0072^{\circ}$ (0.055 - 0.069)	/	0.010 ± 0.0059 (0.012 - 0.023)	0.0051 ± 0.0036 (0.0021 - 0.091)		
$C_{11}H_{13}NO_5$	238.0721	0.26 ± 0.10 (0.11 - 0.41)	0.10 ± 0.036 (0.067 - 0.14)	0.068 ± 0.049 (0.039 - 0.13)	0.021 ± 0.0077 (0.0096 - 0.028)	0.012 ± 0.0026 (0.0092 - 0.015)		
$C_{11}H_{13}NO_6$	254.067	0.011 ± 0.0053 (0.0038 – 0.019)	/	/	0.0016 ± 0.0002 (0.0014 - 0.0018)	/		
Subtotal		2.28 ± 0.87 (0.85 - 3.11)	2.44 ± 0.67 (1.76 – 3.10)	1.00 ± 0.40 (0.59 – 1.38)	0.80 ± 0.23 (0.76 – 1.03)	0.12 ± 0.047 (0.077 – 0.17)		

Table S6. Average and ranges of contribution of identified nitro-aromatic compounds to Abs₃₆₅ of extracted OM (Abs_{365,NAC}%) from laboratory biomass burning samples.

^a Not detected; ^b only detected in one of the three samples; ^c detected in two samples, the value represents average $\pm |x_1 - x_2|/2$.



Figure S1. Extracted ion chromatogram (EIC) of (a) $C_6H_5NO_3$, (b) $C_6H_5NO_4$, (c) $C_7H_7NO_4$, (d) $C_6H_5NO_5$, (e) $C_8H_7NO_4$, (f) $C_8H_9NO_4$, (g) $C_7H_7NO_5$, (h) $C_{10}H_7NO_3$, (i) $C_9H_9NO_4$, (j) $C_8H_9NO_5$, (k) $C_{10}H_{11}NO_4$, (l) $C_{10}H_{11}NO_5$, (m) $C_{11}H_{13}NO_5$ and (n) $C_{11}H_{13}NO_6$ identified in the flaming phase sample collected during NC forest 1 experiment, burn 2 (Table S1).



Figure S1. Continue



Figure S1. Continue



Figure S2. Q-ToF MS/MS spectra of (a) $C_6H_5NO_3$, (b) $C_6H_5NO_4$, (c, d) $C_7H_7NO_4$ isomers (e) $C_6H_5NO_5$, (f, g) $C_8H_7NO_4$ isomers, (h, i) $C_8H_9NO_4$ isomers, (j) $C_7H_7NO_5$, (k) $C_{10}H_7NO_3$, (l, m) $C_9H_9NO_4$ isomers, (n) $C_8H_9NO_5$, (o-q) $C_{10}H_{11}NO_4$ isomers, (r) $C_{10}H_{11}NO_5$, (s) $C_{11}H_{13}NO_5$ and (t) $C_{11}H_{13}NO_6$ identified in the flaming phase sample collected during NC forest 1 experiment, burn 2 (Table S1).



Figure S2. Continue



Figure S2. Continue



Figure S3. Q-ToF MS/MS spectra of standard compounds, (a) 4-nitrophenol, (b) 4-nitrocatechol, (c)2-methyl-4-nitroresorcinol, (d) 2-nitrophloroglucinol, (e) 2-methyl-5-nitrobenzoic acid, (f) 2-nitro-1-naphthol and (g) 2,5-dimethyl-4-nitrobenzoic acid. These MS/MS data were obtained from Xie et al. (2017a).



Figure S4. Linear regressions of (a) MAC₅₅₀ vs. EC/OC with sample data from each experiment, (b) MAC₃₆₅ vs. EC/OC with pooled sample data from all the three experiments, (c) $Å_{abs}$ vs. EC/OC with sample data from each experiment, (d) $Å_{abs}$ vs. EC/OC with pooled sample data from all the three experiments, (e) tNAC_{OM}% vs. EC/OC and (f) Abs_{365,tNAC}% vs. EC/OC with sample data from each experiment.

References

- Chen, Y., and Bond, T. C.: Light absorption by organic carbon from wood combustion, Atmos. Chem. Phys., 10, 1773-1787, 10.5194/acp-10-1773-2010, 2010.
- Hecobian, A., Zhang, X., Zheng, M., Frank, N., Edgerton, E. S., and Weber, R. J.: Water-soluble organic aerosol material and the light-absorption characteristics of aqueous extracts measured over the Southeastern United States, Atmos. Chem. Phys., 10, 5965-5977, 10.5194/acp-10-5965-2010, 2010.
- Laskin, A., Laskin, J., and Nizkorodov, S. A.: Chemistry of atmospheric brown carbon, Chem. Rev., 115, 4335-4382, 10.1021/cr5006167, 2015.
- Xie, M., Chen, X., Hays, M. D., Lewandowski, M., Offenberg, J., Kleindienst, T. E., and Holder, A. L.: Light absorption of secondary organic aerosol: composition and contribution of nitroaromatic compounds, Environ. Sci. Technol., 51, 11607-11616, 10.1021/acs.est.7b03263, 2017a.
- Xie, M., Hays, M. D., and Holder, A. L.: Light-absorbing organic carbon from prescribed and laboratory biomass burning and gasoline vehicle emissions, Sci. Rep., 7, 7318, 10.1038/s41598-017-06981-8, 2017b.