

Table S1: Parameters used to calculate gas-particle partitioning by absorption theory at three different values of activity coefficients (\mathcal{E}), each of 0.3, 1, and 3 (Seinfeld and Pankow, 2003), representing the upper, middle, and lower range of calculated fraction in the particle phase (F_p), respectively. Subcooled vapour pressures were obtained from the Estimation Programs Interface suite (EPA, 2012). The vapour pressure values were corrected for average ambient temperature during sample collection (282 K) using Clausius-Clapeyron equation, then the corrected values were used to calculate the partitioning coefficient, expressed F_p .

Compound	Number of carbon atoms	Molecular mass (g mol ⁻¹)	Subcooled vapour pressure at 298.15 K (atm)	Enthalpy of vaporization (kJ mol ⁻¹)	Partitioning coefficient at $\mathcal{E}=1$ (m ³ μg ⁻¹)	Calculated (F_p)		
						$\mathcal{E}=0.3$	$\mathcal{E}=1$	$\mathcal{E}=3$
Naphthalene	10	128.18	3.93×10^{-4}	60.3 ^a	1.82×10^{-06}	1.4×10^{-5}	4.2×10^{-6}	1.4×10^{-6}
Acenaphthene	12	154.21	1.34×10^{-5}	70.5 ^a	5.62×10^{-5}	4.4×10^{-4}	1.3×10^{-4}	4.4×10^{-5}
Anthracene	14	178.24	6.50×10^{-7}	79.5 ^a	1.23×10^{-3}	9.5×10^{-3}	2.9×10^{-3}	9.6×10^{-4}
Pyrene	16	202.26	1.05×10^{-7}	87.5 ^a	8.11×10^{-3}	5.9×10^{-2}	1.9×10^{-2}	6.3×10^{-3}
Benzo(ghi)fluoranthene	18	226.28	4.60×10^{-9}	65.2 ^a	9.89×10^{-2}	0.43	0.19	0.07
Benzo(a)pyrene	20	252.32	2.28×10^{-10}	105 ^a	4.45	0.97	0.91	0.78
Picene	22	278.36	1.19×10^{-11}	135 ^a	153.34	1.00	1.00	0.99
Phthalic anhydride	8	148.12	7.57×10^{-6}	52.9 ^b	6.94×10^{-5}	5.4×10^{-4}	1.6×10^{-4}	5.4×10^{-5}
Phthalic acid	8	166.13	8.91×10^{-8}	74.1 ^b	8.54×10^{-3}	6.2×10^{-2}	2.0×10^{-2}	6.6×10^{-3}
Isophthalic acid	8	166.13	1.61×10^{-7}	84.3 ^b	5.97×10^{-3}	4.4×10^{-2}	1.4×10^{-2}	4.6×10^{-3}
Terephthalic acid	8	166.13	1.22×10^{-7}	93.4 ^b	9.67×10^{-3}	7.0×10^{-2}	2.2×10^{-2}	7.5×10^{-3}
2,5-Furandione	4	98.06	6.19×10^{-4}	56.7 ^c	3.80×10^{-7}	3.0×10^{-6}	8.8×10^{-7}	3.0×10^{-7}
Dihydro-2,5-furandione	4	100.07	1.15×10^{-5}	57.3 ^c	2.00×10^{-5}	1.6×10^{-5}	4.6×10^{-5}	1.6×10^{-6}
3-Methyl-2,5-furandione	5	112.08	2.22×10^{-4}	53.1 ^c	9.29×10^{-7}	7.2×10^{-6}	2.1×10^{-6}	7.2×10^{-7}
Dihydro-3-methyl-2,5-furandione	5	114.09	4.98×10^{-5}	59.3 ^c	4.07×10^{-6}	3.2×10^{-5}	9.4×10^{-6}	3.2×10^{-7}

^a (Kluwer, 1988), ^b (Yaws, 2009), ^c (Linstrom, 2005)

Table S2: Mass spectral fragmentations for trimethylsilylated derivatives of the nitromonoaromatic compounds using electron impact ionization (70 eV). Base peaks were used for quantification, and other fragments were used as qualifiers. Results are listed according to the observed intensities (highest to lowest).

Nitromonoaromatics	Molecular mass (g mol ⁻¹)	Calculated der. mass (g mol ⁻¹)	MS Fragments (<i>m/z</i>)					
			Base peak	1	2	3	4	5
4-Nitrophenol 2,3,5,6-D ₄ (IS)	143.13	215.13	200	215	154	139	73	45
4-Nitrophenol	139.11	211.11	196	211	150	135	73	45
4-Nitrocatechol	155.11	299.11	284	299	73	45		
4-Methyl-5-nitrocatechol	169.13	313.13	313	73	296	266	180	45
4-Nitroguaiacol	169.13	241.13	211	226	241	181	73	45
5-Nitroguaiacol	169.13	241.13	211	226	241	181	73	45
4-Methyl-2-nitrophenol	153.14	225.14	210	165	179	73	225	45
5-Methyl-2-nitrophenol	153.14	225.14	210	165	179	73	45	225
4-Methyl-3-nitrophenol	153.14	225.14	208	163	225	180	73	45
2-Methyl-4-nitrophenol	153.14	225.14	210	225	164	149	73	45
4-Hydroxy-3-nitrobenzyl alcohol	169.14	313.14	298	224	147	179	313	45
4-Methoxy-2-nitrophenol	169.13	241.13	226	181	241	153	73	45
3-Nitrosalicylic acid-D ₃	186.14	330.14	315	73	147	236	329	45
5-Nitrosalicylic acid	183.12	327.12	312	73	45	326		

Table S3: Spearman's correlation coefficients (r_s) for PM_{2.5} tracer concentrations reported in this study (n=14).

	DHOPA	PhA	i-PhA	t-PhA	4M-PhA	4NP	4M-2NP	2M-4NP	4NG	4NC	4M-5NC	4H-3NB	5NSA	Furandiones ^a	Hopanes ^b	Levoglucosan
DHOPA	x															
PhA	0.7	x														
i-PhA	0.8	0.6	x													
t-PhA	0.6	0.5	0.9	x												
4M-PhA	0.8	0.7	0.7	0.5	x											
4NP	0.2	0.1	0.3	0.4	0.4	x										
4M-2NP	0.1	0.3	0.2	0.4	0.4	0.2	x									
2M-4NP	0.4	0.1	0.3	0.4	0.5	0.8	0.4	x								
4NG	0.1	0.2	0.4	0.3	0.0	-0.1	0.1	-0.1	x							
4NC	0.1	0.1	0.7	0.9	0.2	0.1	0.2	0.0	0.2	x						
4M-5NC	0.2	0.3	0.7	0.9	0.3	0.2	0.5	0.1	0.4	0.9	x					
4H-3NB	0.3	0.2	0.5	0.4	-0.1	-0.2	0.2	0.1	0.5	0.4	0.5	x				
5NSA	0.5	0.6	0.7	0.8	0.6	0.4	0.2	0.4	0.2	0.7	0.7	0.0	x			
Furandiones ^a	0.5	0.5	0.2	-0.2	0.6	0.0	-0.2	0.0	0.1	-0.5	-0.4	-0.1	-0.2	x		
Hopanes ^b	0.2	0.2	0.6	0.8	0.2	0.3	0.3	0.2	0.1	0.9	0.8	0.1	0.9	-0.6	x	
Levoglucosan	0.3	0.4	0.7	0.7	0.3	0.2	0.0	-0.1	0.4	0.9	0.9	0.2	0.8	-0.2	0.8	x

 p – value ≤ 0.001
 p – value 0.01 - 0.001
 p – value ≤ 0.05 and > 0.01
Bolded when $r_s \geq 0.4$

^a Furandiones correspond to the sum of 2,5-furandione (FD), dihydro-2,5-furandione(DFD), 3-methyl-2,5-furandione(MFD), and dihydro-3-methyl-2,5-furandione(DMFD).

^b Hopanes correspond to the sum of 17 α (H)-22,29,30-trisnorhopane, 17 β (H)-21 α (H)-30-norhopane, and 17 α (H)-21 β (H)-hopane.

Table S4: Daily measurements of organic carbon (OC), elemental carbon (EC), ambient temperature and relative humidity (RH), in Iowa City, IA from Nov 4 - Nov. 17, 2011.

	OC ($\mu\text{g m}^{-3}$) Average \pm SD	EC ($\mu\text{g m}^{-3}$) Average \pm SD	Average daily Temperature ($^{\circ}\text{C}$)	RH (%)
11/4/2015	1.76 \pm 0.10	0.14 \pm 0.02	14	87
11/5/2015	0.66 \pm 0.05	0.11 \pm 0.02	15	85
11/6/2015	1.12 \pm 0.07	0.11 \pm 0.02	7	72
11/7/2015	2.28 \pm 0.12	0.25 \pm 0.02	5	68
11/8/2015	1.95 \pm 0.11	0.26 \pm 0.02	5	68
11/9/2015	2.90 \pm 0.15	0.38 \pm 0.03	5	65
11/10/2015	3.01 \pm 0.16	0.26 \pm 0.02	6	70
11/11/2015	1.95 \pm 0.11	0.13 \pm 0.02	11	81
11/12/2015	1.07 \pm 0.07	0.03 \pm 0.02	6	74
11/13/2015	1.56 \pm 0.09	0.18 \pm 0.02	4	57
11/14/2015	2.12 \pm 0.12	0.13 \pm 0.02	8	66
11/15/2015	9.65 \pm 0.49	0.81 \pm 0.04	10	59
11/16/2015	1.37 \pm 0.08	0.10 \pm 0.02	9	72
11/17/2015	1.23 \pm 0.08	0.05 \pm 0.02	13	95

Figure S1: Mass spectrum of phthalic anhydride (a) and phthalic acid (b), injected directly to a GCMS system equipped with a Carbowax column and an inlet heated to 250 °C. Both species eluted at the same retention time (13.46 min) and exhibited the same mass spectra, with m/z 148 being the molecular ion for phthalic anhydride. Phthalic acid likely dehydrates (loses H₂O) in the GC the injection port forming its anhydride derivative. The trimethylsilylated derivatives mass spectra for phthalic anhydride (c) and phthalic acid (d) also had identical retention times (13.45 min) and exhibited identical mass spectra, with m/z 310 being the molecular ion for the derivatized product.

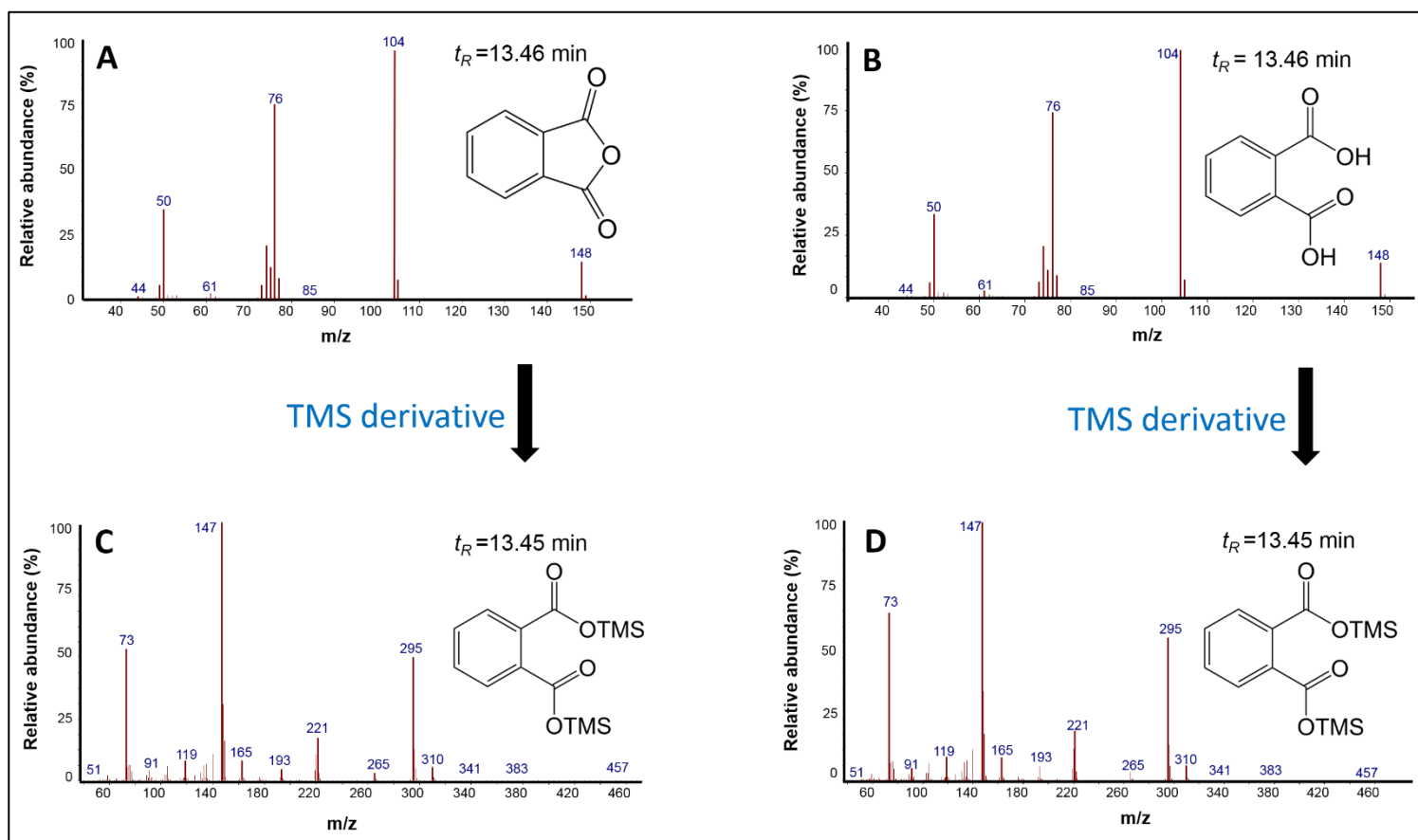


Figure S2: The daily distribution of the detected nitromonoaromatics between gas and particle phases. The phase distributions of 4-nitrocatechol and 4-methyl-5-nitrocatechol are not shown in this figure due to the low extraction efficiency.

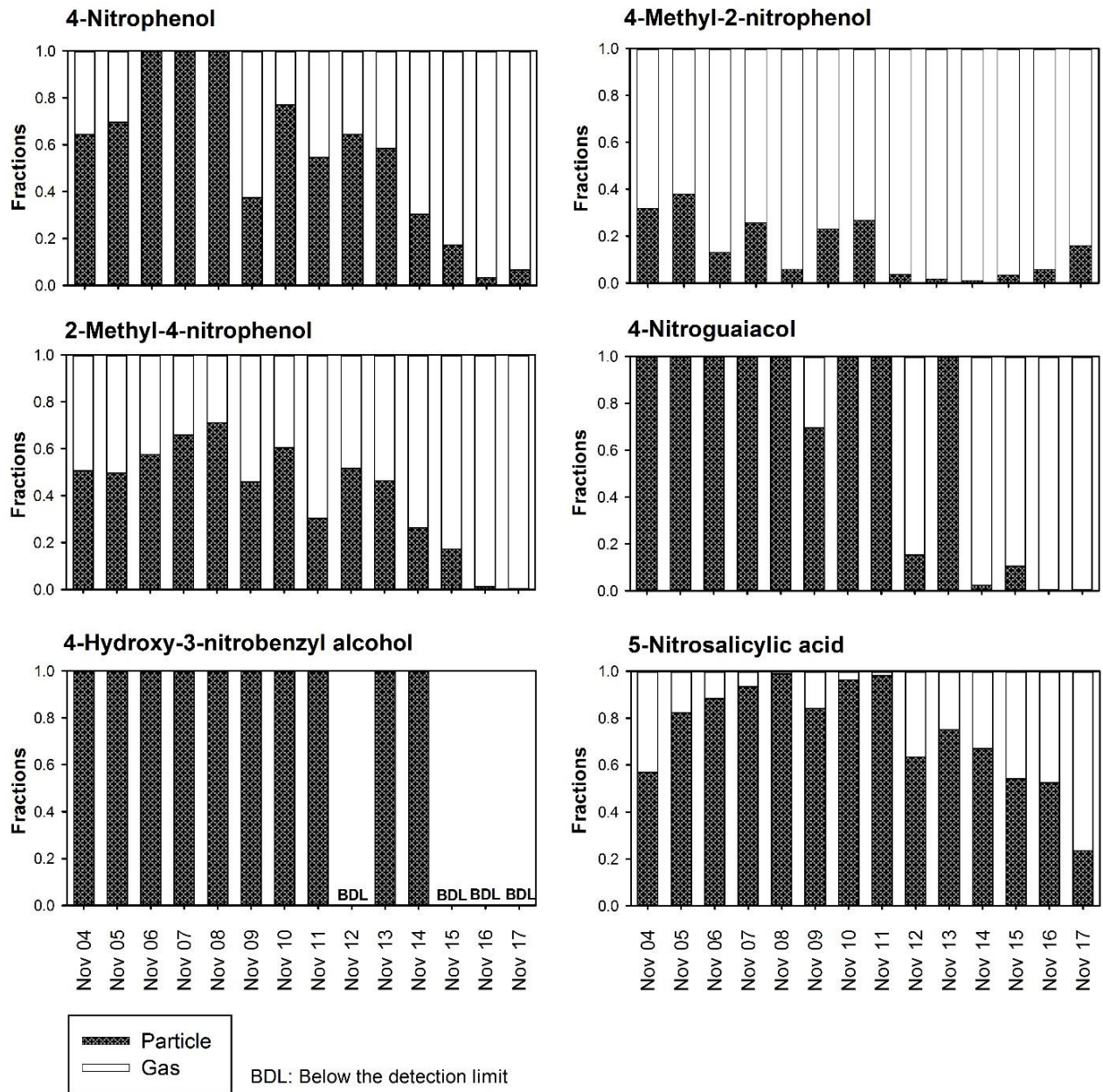


Figure S3: Daily gas and particle concentrations of select nitroaromatics detected in Iowa City during fall 2015, including 4-nitrophenol (4NP), 4-methyl-2-nitrophenol (4M-2NP), 2-methyl-4-nitrophenol (2M-4NP), 4-nitroguaiacol (4NG), and 4-hydroxy-3-nitrobenzyl alcohol (4H-3NB).

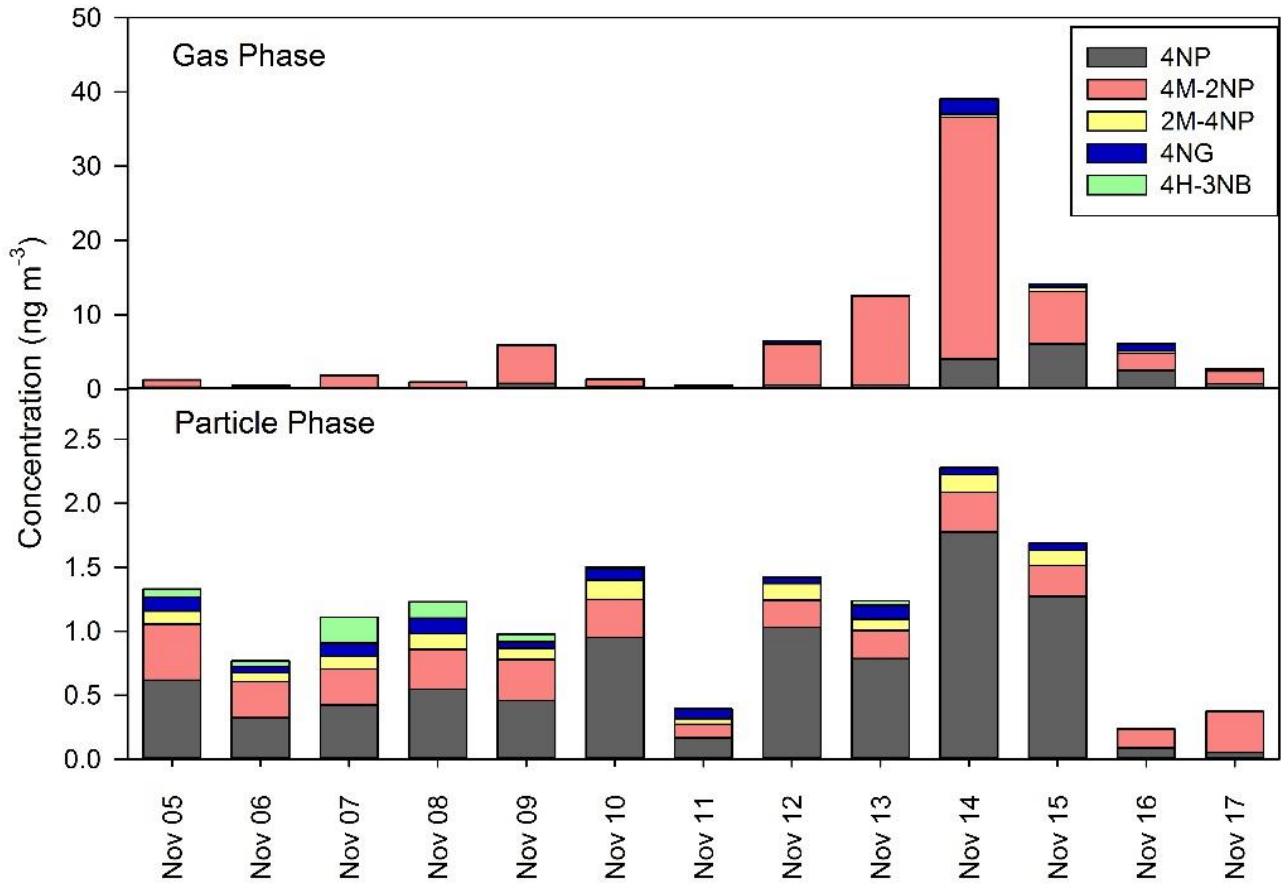
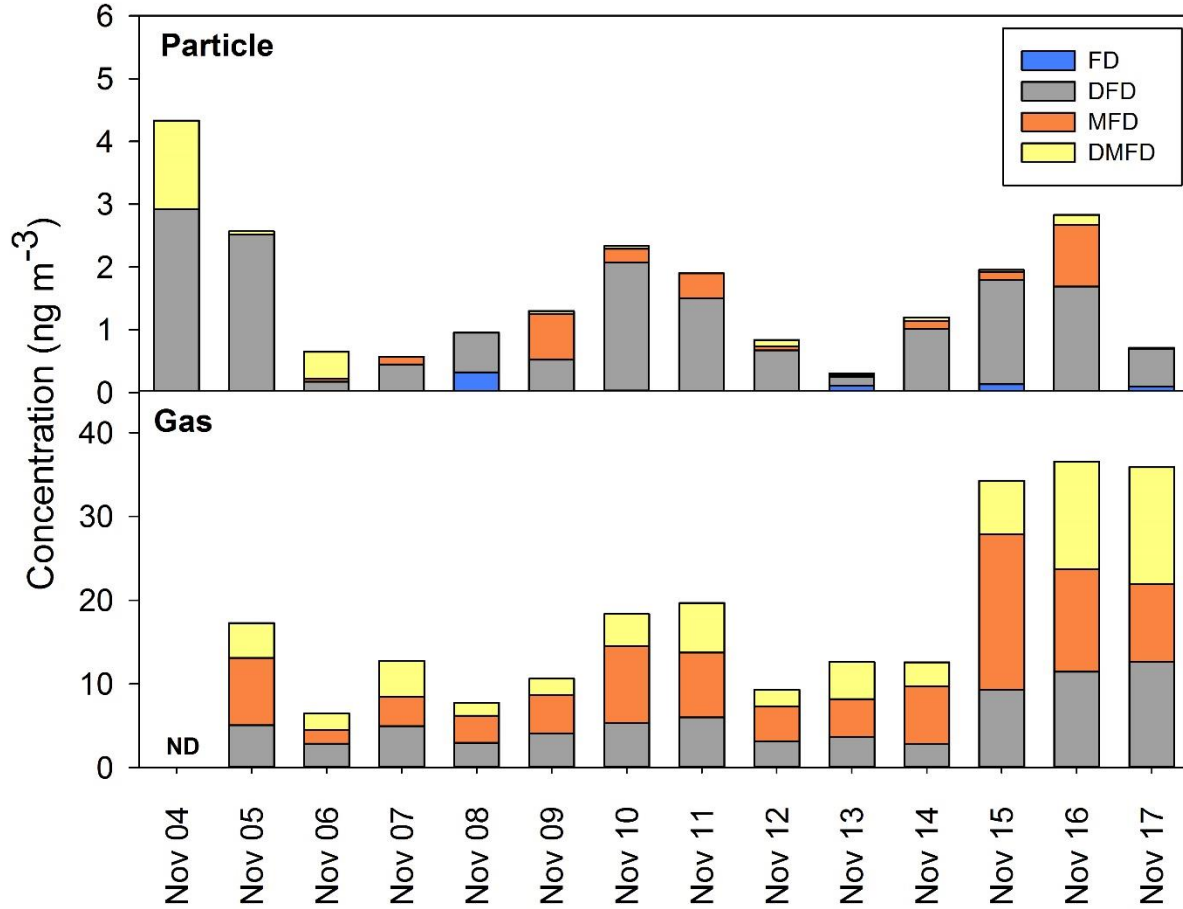


Figure S4: Ambient concentrations for individual furandiones detected in gas and particle phases. Furandiones were not detected in gas phase on 4 November. Gas phase concentrations were corrected to the average recovery (n=3) of authentic standards from the PUF ($38.4 \pm 2.8\%$ for DFD, $31.8 \pm 2.6\%$ for MFD, and $44.2 \pm 2.7\%$ for DMFD).



Works Cited

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