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Contributions of primary emissions and secondary formation to nitrated aromatic compounds in the mountain background region of Southeast China

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Table S1 Limit of detection (LOD) and concentrations in blank samples of the target compounds in this study.

Compounds[a]	m/z[b]	LOD (ng μL^{-1})	Concentrations in blank samples (ng m^{-3})			
			Spring	Summer	Autumn	Winter
4NP	196	0.000407	NA[c]	NA[c]	0.046824	0.018609
3M4NP	210	0.000109	NA[c]	NA[c]	NA[c]	0.000757
4NGA	211	0.001422	0.001549	0.003857	0.005888	0.002407
5NGA	211	0.001209	0.003656	0.000730	0.003529	NA[c]
4NC	284	0.006847	NA[c]	NA[c]	NA[c]	NA[c]
2,4-DNP	241	0.006842	0.017479	0.008151	0.002099	NA[c]
4M5NC	313	0.000233	0.073688	0.054543	0.034838	0.012273
3NSA	312	0.000337	0.000362	NA[c]	NA[c]	NA[c]
5NSA	312	0.000261	NA[c]	NA[c]	NA[c]	NA[c]

[a]4NP:4-nitrophenol; 3M4NP:3-methyl-4-nitrophenol; 2,4-DNP:2,4-dinitrophenol; 4NGA:4-nitroguaiacol; 5NGA:5-nitroguaiacol;4NC:4-nitrocatechol; 4M5NC:4-methyl-5-nitrocatechol; 3NSA:3-nitrosalicylic acid; 5NSA:5-nitrosalicylic acid.

[b] Mass-to-charge ratio of fragment ions for qualification and quantification.

[c] NA: not available.

Table S2 Values of *Q* (robust), *Q* (true) and average r^2 for the modeling results in the whole sampling period.

species	the whole sampling period
Q (robust)	2120
Q (true)	2270
SO_2(r^2)	0.948
NO_2(r^2)	0.837
O_3(r^2)	0.586
SO_4^{2-}(r^2)	0.958
NO_3^-(r^2)	0.933
NH_4^+(r^2)	0.962
K^+(r^2)	0.905
ff-*n*-alkanes(r^2)	0.915
PAHs(r^2)	0.934
levoglucosan(r^2)	0.962
4NP(r^2)	0.962
3M4NP(r^2)	0.512
4NGA(r^2)	0.692
5NGA(r^2)	0.796
4NC(r^2)	0.852
4M5NC(r^2)	0.715
3NSA(r^2)	0.871
5NSA(r^2)	0.954

Table S3. Pearson correlations between individual NAC species and meteorological parameters, aerosol components, and gas pollutants during spring (n = 11).

	NACs	4NP	3M4NP	2,4-DNP	4NGA	5NGA	4NC	4M5NC	3NSA	5NSA
$PM_{2.5}$	0.818**	0.803**	0.655*	0.165	0.594	0.756**	0.713*	0.880**	0.648*	0.684*
SO_2	0.736**	0.789**	0.874**	0.234	0.126	0.386	0.714*	0.630*	0.700*	0.696*
NO_2	0.945**	0.930**	0.457	(0.037)	0.115	0.803**	0.950**	0.709*	0.934**	0.943**
O_3	0.783**	0.805**	0.855**	0.245	0.275	0.588	0.704*	0.803**	0.665*	0.684*
ff- *n*-alkanes	0.736**	0.704*	0.526	0.607*	0.215	0.481	0.690*	0.640*	0.721*	0.716*
PAHs	0.794**	0.826**	0.612*	(0.039)	0.261	0.562	0.772**	0.668*	0.748**	0.784**
Levoglucosan	0.933**	0.936**	0.422	0.122	(0.115)	0.621*	0.975**	0.684*	0.985**	0.966**
K^+	0.780**	0.766**	0.454	0.158	0.416	0.664*	0.705*	0.818**	0.679*	0.706*
SO_4^{2-}	0.545	0.535	0.6	0.336	0.609*	0.458	0.422	0.773**	0.36	0.382
NO_3^-	0.790**	0.786**	0.113	(0.093)	(0.202)	0.574	0.860**	0.468	0.883**	0.890**
NH_4^+	0.701*	0.696*	0.662*	0.354	0.561	0.564	0.592	0.822**	0.543	0.569

**Significant correlation at the 0.01 level.

*Significant correlation at the 0.05 level.

Red data in parentheses represent negative values.

Table S4. Pearson correlations between individual NAC species and meteorological parameters, aerosol components, and gas pollutants during summer (n = 13).

	NACs	4NP	3M4NP	2,4-DNP	4NGA	5NGA	4NC	4M5NC	3NSA	5NSA
$PM_{2.5}$	0.875**	0.940**	0.619*	0.058	0.679*	0.749**	0.926**	0.759**	0.820**	0.930**
SO_2	0.859**	0.794**	0.585*	0.267	0.585*	0.763**	0.889**	0.819**	0.743**	0.823**
NO_2	0.869**	0.865**	0.537	0.311	0.629*	0.697**0	0.929**	0.863**	0.866**	0.834**
O_3	0.786**	0.836**	0.426	0.028	0.553*	0.666*	0.877**	0.740**	0.763**	0.799**
ff- *n*-alkanes	0.852**	0.861**	0.701**	0.199	0.805**	0.732**	0.846**	0.718**	0.732**	0.856**
PAHs	0.880**	0.916**	0.628*	0.196	0.692**	0.739**	0.898**	0.807**	0.837**	0.892**
Levoglucosan	0.731**	0.52	0.515	0.616*	0.716**	0.669*	0.651*	0.697**	0.682*	0.504
K^+	0.827**	0.914**	0.485	0.095	0.606*	0.676*	0.894**	0.768**	0.842**	0.860**
SO_4^{2-}	0.884**	0.968**	0.639*	0.03	0.707**	0.782**	0.895**	0.738**	0.837**	0.952**
NO_3^-	0.678*	0.654*	0.281	0.244	0.393	0.511	0.799**	0.774**	0.690**	0.612*
NH_4^+	0.881**	0.966**	0.637*	0.032	0.722**	0.774**	0.894**	0.737**	0.836**	0.945**

**Significant correlation at the 0.01 level.

*Significant correlation at the 0.05 level.

Red data in parentheses represent negative values.

Table S5. Pearson correlations between individual NAC species and meteorological parameters, aerosol components, and gas pollutants during autumn (n = 13).

	NACs	4NP	3M4NP	2,4-DNP	4NGA	5NGA	4NC	4M5NC	3NSA	5NSA
$PM_{2.5}$	0.684**	0.715**	0.211	(0.02)	0.240	0.467	0.409	0.768**	0.393	0.660*
SO_2	0.805**	0.847**	0.031	(0.169)	(0.016)	0.211	0.659*	0.633*	0.177	0.838**
NO_2	0.886**	0.932**	(0.286)	(0.002)	(0.255)	0.026	0.823**	0.588*	0.173	0.899**
O_3	0.165	0.227	(0.104)	(0.316)	0.115	0.258	(0.028)	0.482	0.38	0.145
ff- *n*-alkanes	0.943**	0.932**	(0.16)	0.296	(0.082)	0.225	0.844**	0.647*	0.174	0.894**
PAHs	0.886**	0.879**	(0.135)	0.124	(0.119)	0.153	0.825**	0.533	0.043	0.901**
Levoglucosan	0.888**	0.809**	(0.351)	0.090	(0.143)	0.223	0.847**	0.696**	0.207	0.799**
K^+	0.808**	0.799**	(0.052)	0.012	0.111	0.379	0.616*	0.771**	0.318	0.773**
SO_4^{2-}	0.615*	0.636*	0.29	(0.1)	0.304	0.475	0.354	0.730**	0.266	0.592*
NO_3^-	0.700**	0.889**	0.143	0.078	(0.090)	0.02	0.53	0.374	0.084	0.801**
NH_4^+	0.715**	0.760**	0.172	(0.128)	0.178	0.407	0.471	0.729**	0.287	0.720**

**Significant correlation at the 0.01 level.

*Significant correlation at the 0.05 level.

Red data in parentheses represent negative values.

Table S6. Pearson correlations between individual NAC species and meteorological parameters, aerosol components, and gas pollutants during winter (n = 12).

	NACs	4NP	3M4NP	2,4-DNP	4NGA	5NGA	4NC	4M5NC	3NSA	5NSA
$PM_{2.5}$	0.710**	0.768**	0.324	0.674*	0.262	0.553	0.456	0.628*	0.592*	0.539
SO_2	0.659*	0.749**	0.671*	0.241	(0.190)	(0.229)	0.485	0.33	0.509	0.755**
NO_2	0.879**	0.720**	0.687*	0.557	(0.168)	0.095	0.901**	0.108	0.712**	0.611*
O_3	0.55	0.567	0.114	0.311	0.281	0.582*	0.284	0.718**	0.503	0.489
ff- *n*-alkanes	0.790**	0.853**	0.56	0.566	0.313	0.605*	0.504	0.602*	0.751**	0.656*
PAHs	0.817**	0.883**	0.892**	0.358	(0.149)	(0.082)	0.589*	0.4	0.763**	0.896**
Levoglucosan	0.835**	0.692*	0.373	0.484	0.244	0.593*	0.682*	0.562	0.797**	0.605*
K^+	0.768**	0.760**	0.402	0.570	0.359	0.571	0.561	0.552	0.642*	0.571
SO_4^{2-}	0.453	0.625*	0.249	0.659*	0.118	0.328	0.251	0.373	0.271	0.324
NO_3^-	0.56	0.716**	0.524	0.324	(0.047)	(0.013)	0.413	0.258	0.284	0.517
NH_4^+	0.413	0.596*	0.271	0.587*	0.045	0.233	0.243	0.274	0.201	0.299

**Significant correlation at the 0.01 level.

*Significant correlation at the 0.05 level.

Red data in parentheses represent negative values.

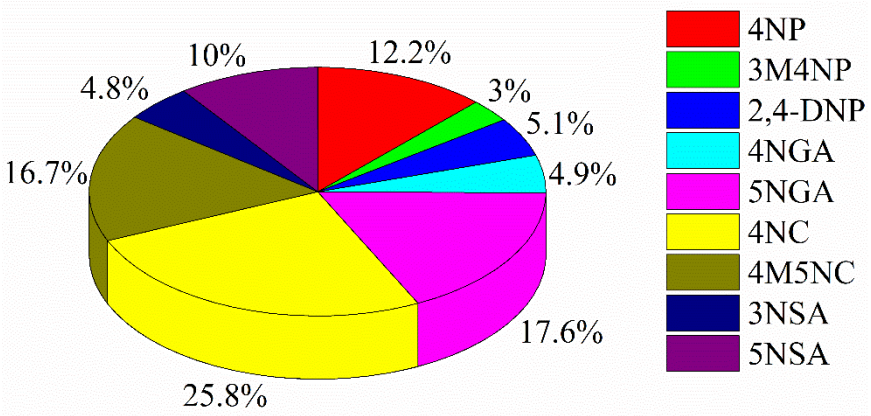

Fig. S1 Relative contribution of each NACs species during the whole year (4NP: 4-nitrophenol; 3M4NP: 3-methyl-4-nitrophenol; 2,4-DNP: 2,4-dinitrophenol; 4NGA: 4-nitroguaiacol; 5NGA: 5-nitroguaiacol;4NC: 4-nitrocatechol; 4M5NC: 4-methyl-5-nitrocatechol; 3NSA: 3-nitrosalicylic acid; 5NSA: 5-nitrosalicylic acid).