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Chemically speciated air pollutant emissions from open burning of household solid waste from South Africa

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S1. $PM_{2.5}$ Mass Closure

Mass closure, a comparison of the reconstructed mass and sum of measured species with gravimetric mass, is an indicator of the data quality. It also provides information about key chemical composition and potential sources of $PM_{2.5}$ (Chow et al., 2015).

Sum of measured species should be less than or equal to the corresponding gravimetric $PM_{2.5}$ mass concentrations because species such as oxygen (O) and hydrogen (H) are not measured. The U.S. Environmental Protection Agency (EPA) Quality Assurance Guidance for $PM_{2.5}$ Chemical Speciation suggests that the ratio of sum of species over gravimetric mass should be within the range of 0.60–1.32 (U.S. EPA, 2012). This sum includes chemicals quantified on the Teflon-membrane and quartz-fiber filters without double counting. Measured concentrations do not account for unmeasured O associated with metal oxides in minerals, unmeasured anions and cations, or H, nitrogen (N), and O associated with organic carbon. Figure S1a shows that the sum of species accounts for 73% of $PM_{2.5}$, which is within the U.S. EPA limit.

Mass reconstruction consists of five major categories, including organic matter (OM = OC × $f_{OM/OC}$), elemental carbon (EC), ions, minerals, and other species (Chow et al., 2015; Watson et al., 2016). Ions include ammonium (NH_4^+), sodium (Na^+), magnesium (Mg^{2+}), potassium (K^+), calcium (Ca^{2+}), fluoride (F^-), chloride (Cl^-), nitrite (NO_2^-), nitrate (NO_3^-), and sulfate (SO_4^{2-}) by IC (Chow and Watson, 2017). Minerals are estimated as 2.2×Al + 2.49×Si + 1.63×Ca + 2.42×Fe + 1.94×Ti, following the IMPROVE formula (Chow et al., 2015; Malm et al., 1994). "Other species" include the measured species not included in the major components without double counting.

The multiplier ($f_{OM/OC}$) for converting organic carbon (OC) to OM varies with the composition of OM, ranging from 1.2 for fresh vehicle engine emissions (Kleeman et al., 2000) and fresh urban aerosols (Chow et al., 2002) to 2.6 for aged aerosols (Turpin and Lim, 2001). A value of 1.4 has been most commonly used for urban aerosols, and a value of 1.8 is used for more aged non-urban aerosols (Chow et al., 2015). Reid et al. (2005) found the $f_{OM/OC}$ value to be ~1.5 for fresh biomass burning smoke. Assuming that all species are measured and analytical uncertainties are negligible, $f_{OM/OC}$ values for different materials can be estimated from mass closure as (Pani et al., 2019):

$$f_{OM/OC} = \frac{PM_{2.5} - EC - Ions - Minerals - Others}{OC} \quad \text{(S1)}$$

Table S1 shows that $f_{OM/OC}$ varies from 1.22 for dry vegetation to 1.87 for food discard, with smoldering materials (except rubber) having higher values than flaming materials, indicating more oxygen in organic aerosols from smoldering combustions. The overall average $f_{OM/OC}$ value for all test conditions is 1.4, which is used to convert OC to OM in mass reconstruction.

Figure S1b compares reconstructed with gravimetric masses showing a linear regression slope of 0.99. Note that some data points have reconstructed masses higher or lower than gravimetric mass, likely due to uncertainties in the estimation of OM and minerals as well as potential positive and negative sampling artifacts. The differences between gravimetric and reconstructed masses are referred to as unidentified species. Because the mass closure has ratios close to unity based on both sum of species and reconstructed mass, the chemical analysis of major $PM_{2.5}$ constituents (i.e., gravimetric mass, carbon, ions, and elements) are of high quality.

Table S1: Measured organic matter (OM) to organic carbon (OC) ratio ($f_{OM/OC}$).

Material	$f_{OM/OC}$
Paper	1.66 ± 0.16
Rubber	1.27 ± 0.07
Textile	1.36 ± 0.28
Plastic (Bottles)	1.42 ± 0.02
Plastic (Bags)	1.66 ± 0.60
Vegetation (0%)	1.22 ± 0.11
Vegetation (20%)	1.38 ± 0.15
Vegetation (50%)	1.63 ± 0.12
Food Discards	1.87 ± 0.09
Combined	1.40 ± 0.21

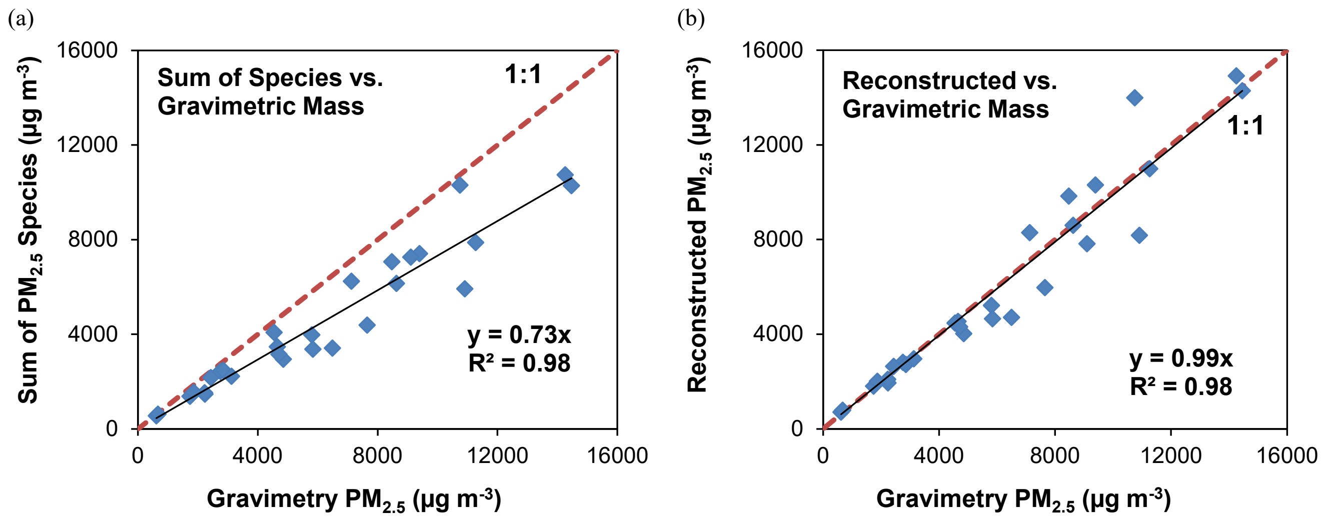


Figure S1: Comparison of: (a) sum of species and (b) reconstructed mass with gravimetric mass of $PM_{2.5}$.

S2. Supplementary Tables

Table S2: Comparison of heavy metal emission factors (mg kg^{-1} fuel) between this study and those from other published measurements.

Element	Cr	Ni	Cu	Zn	Cd	Pb
Paper						
This study	**0.22 ± 0.34**	**0.00 ± 0.06**	**4.30 ± 2.79**	**0.91 ± 0.74**	**0.00 ± 0.77**	**1.70 ± 1.30**
(Park et al., 2013)	0.33–0.38	0.20–0.26	0.07–0.22	0–18.19	0.02–0.05	0–0.07
(Cheng et al., 2020)	0.43–0.69	0.54–0.74	6.17–6.96	1.20–2.09	0.27–0.37	1.83–1.99
Plastics						
This study (bottle)	**4.75 ± 1.91**	**0.00 ± 0.94**	**5.81 ± 9.72**	**0.27 ± 3.17**	**0.52 ± 12.42**	**12.53 ± 10.99**
This study (bag)	**0.26 ± 0.24**	**0.00 ± 0.07**	**3.36 ± 1.01**	**0.99 ± 0.40**	**0.00 ± 0.92**	**1.77 ± 0.88**
(Park et al., 2013)	0.36–1.46	0.05–0.24	0.04–0.12	0–65.17	0.01–0.02	0.002–1.13
(Cheng et al., 2020)	0.49–0.80	0.48–0.62	7.02–8.0	1.66–3.73	0.28–0.45	1.14–1.33
Vegetations						
This study (0%)	**0.26 ± 0.45**	**0.00 ± 0.06**	**0.86 ± 0.75**	**0.41 ± 1.47**	**0.39 ± 0.58**	**0.50 ± 0.74**
This study (20%)	**0.64 ± 0.16**	**0.04 ± 0.08**	**0.35 ± 0.49**	**1.18 ± 3.37**	**0.00 ± 0.45**	**0.87 ± 0.48**
This study (50%)	**5.94 ± 1.33**	**0.24 ± 0.68**	**5.01 ± 3.50**	**2.13 ± 27.22**	**0.00 ± 3.63**	**8.37 ± 2.15**
(Park et al., 2013)	0.14–0.46	0.07–0.50	0.05–0.18	2.69–15.65	0.01–0.19	0.05–0.10
(Cheng et al., 2020)	0.27–0.31	0.34–0.38	5.38–5.45	0.85–2.13	0.18–0.23	1.03–1.21
Combined Materials						
This study	**0.00 ± 0.06**	**0.00 ± 0.03**	**1.53 ± 0.30**	**0.56 ± 0.53**	**0.07 ± 0.41**	**5.59 ± 4.55**
(Lemieux, 1997)	0.176–0.237	0.188–0.804	0.573–15.02	0.073–18.9	0.037–0.239	0.22–2.57
(Christian et al., 2010)			0.35–2.13	0.98–1.72	0.27–0.59	4.0–7.8
(Park et al., 2013)	0.53–1.02	0.15–0.66	0.04–0.08	13.29–14.16	0.01–0.02	0.01–0.05
(Jayarathne et al., 2018)			0.29 ± 0.07		0.07 ± 0.15	4.2 ± 5.7
(Cheng et al., 2020)	0.41–0.62	0.46–0.53	6.55–6.84	1.06–2.44	0.27–0.35	1.12–1.25

Table S3: PAH diagnostic ratios.

Diagnostic ratios	Paper	Rubber	Textile	Plastic (Bottles)	Plastic (Bags)	Vegetation (0%)	Vegetation (20%)	Vegetation (50%)	Food	Combined
FL/(FL+PYR)	0.09 ± 0.03	0.39 ± 0.09	0.14 ± 0.02	0.18 ± 0.06	0.19 ± 0.05	0.12 ± 0.06	0.12 ± 0.02	0.18 ± 0.01	0.10 ± 0.03	0.20 ± 0.04
PHE/ANT	0.41 ± 0.05	0.52 ± 0.02	0.52 ± 0.03	1.10 ± 0.08	1.49 ± 0.53	0.36 ± 0.04	0.76 ± 0.11	0.82 ± 0.06	16.14 ± 3.15	0.93 ± 0.11
ANT/(ANT+PHE)	0.71 ± 0.03	0.66 ± 0.01	0.66 ± 0.01	0.48 ± 0.02	0.41 ± 0.08	0.74 ± 0.02	0.57 ± 0.03	0.55 ± 0.02	0.06 ± 0.01	0.52 ± 0.03
FLA/PYR	1.27 ± 0.19	1.98 ± 0.67	1.31 ± 0.21	2.22 ± 1.31	1.81 ± 0.48	1.21 ± 0.40	1.04 ± 0.11	1.09 ± 0.43	0.81 ± 0.29	1.57 ± 0.10
FLA/(FLA+PYR)	0.56 ± 0.04	0.65 ± 0.07	0.56 ± 0.04	0.66 ± 0.12	0.64 ± 0.06	0.54 ± 0.09	0.51 ± 0.03	0.51 ± 0.10	0.44 ± 0.10	0.61 ± 0.02
BaA/CHR	2.17 ± 0.23	0.36 ± 0.10	2.00 ± 0.19	0.61 ± 0.22	0.57 ± 0.09	1.91 ± 0.95	1.46 ± 0.45	0.92 ± 0.41	1.98 ± 0.88	0.65 ± 0.12
BaA/(BaA+CHR)	0.68 ± 0.02	0.26 ± 0.05	0.67 ± 0.02	0.37 ± 0.08	0.36 ± 0.04	0.63 ± 0.12	0.59 ± 0.07	0.47 ± 0.11	0.65 ± 0.10	0.39 ± 0.05
PYR/BaP	6.17 ± 0.79	0.19 ± 0.02	4.48 ± 1.30	0.26 ± 0.04	0.24 ± 0.08	2.50 ± 0.78	1.06 ± 0.15	1.39 ± 0.08	2.04 ± 0.56	0.67 ± 0.29
BaP/(BaP+CHR)	0.22 ± 0.07	0.27 ± 0.05	0.26 ± 0.05	0.37 ± 0.14	0.41 ± 0.06	0.56 ± 0.12	0.52 ± 0.10	0.36 ± 0.04	0.53 ± 0.09	0.39 ± 0.04
BeP/BaP	1.00 ± 0.07	1.48 ± 0.52	1.45 ± 0.25	3.23 ± 0.86	2.76 ± 0.51	0.85 ± 0.07	1.04 ± 0.12	1.07 ± 0.18	0.92 ± 0.07	1.63 ± 0.30
BaP/BghiP	0.72 ± 0.16	0.82 ± 0.32	0.62 ± 0.10	0.42 ± 0.12	0.43 ± 0.16	0.57 ± 0.13	0.56 ± 0.06	0.49 ± 0.03	0.51 ± 0.11	0.76 ± 0.14
IcdP/BghiP	0.29 ± 0.09	2.23 ± 0.47	0.28 ± 0.14	3.22 ± 1.03	2.86 ± 1.07	0.31 ± 0.08	1.04 ± 0.36	0.91 ± 0.11	1.15 ± 0.30	2.45 ± 0.48
IcdP/(IcdP+BghiP)	0.22 ± 0.05	0.69 ± 0.05	0.21 ± 0.09	0.75 ± 0.07	0.72 ± 0.09	0.23 ± 0.05	0.50 ± 0.09	0.48 ± 0.03	0.53 ± 0.07	0.71 ± 0.04
RET/(RET+CHR)	0.74 ± 0.08	0.00 ± 0.00	0.78 ± 0.07	0.00 ± 0.00	0.00 ± 0.00	0.55 ± 0.09	0.39 ± 0.09	0.31 ± 0.06	0.57 ± 0.04	0.21 ± 0.09

PAH abbreviations:
ANT: Anthracene; BaA: Benzo[a]anthracene; BaP: Benzo[a]pyrene; BeP: Benzo[e]pyrene
BghiP: Benzo[g,h,i]perylene; CHR: Chrysene; FL: Fluorene; FLA: Fluoranthene
IcdP: Indeno[1,2,3-c,d]pyrene; PHE: Phenanthrene; PYR: Pyrene; RET: retene

S3. Supplementary Figures

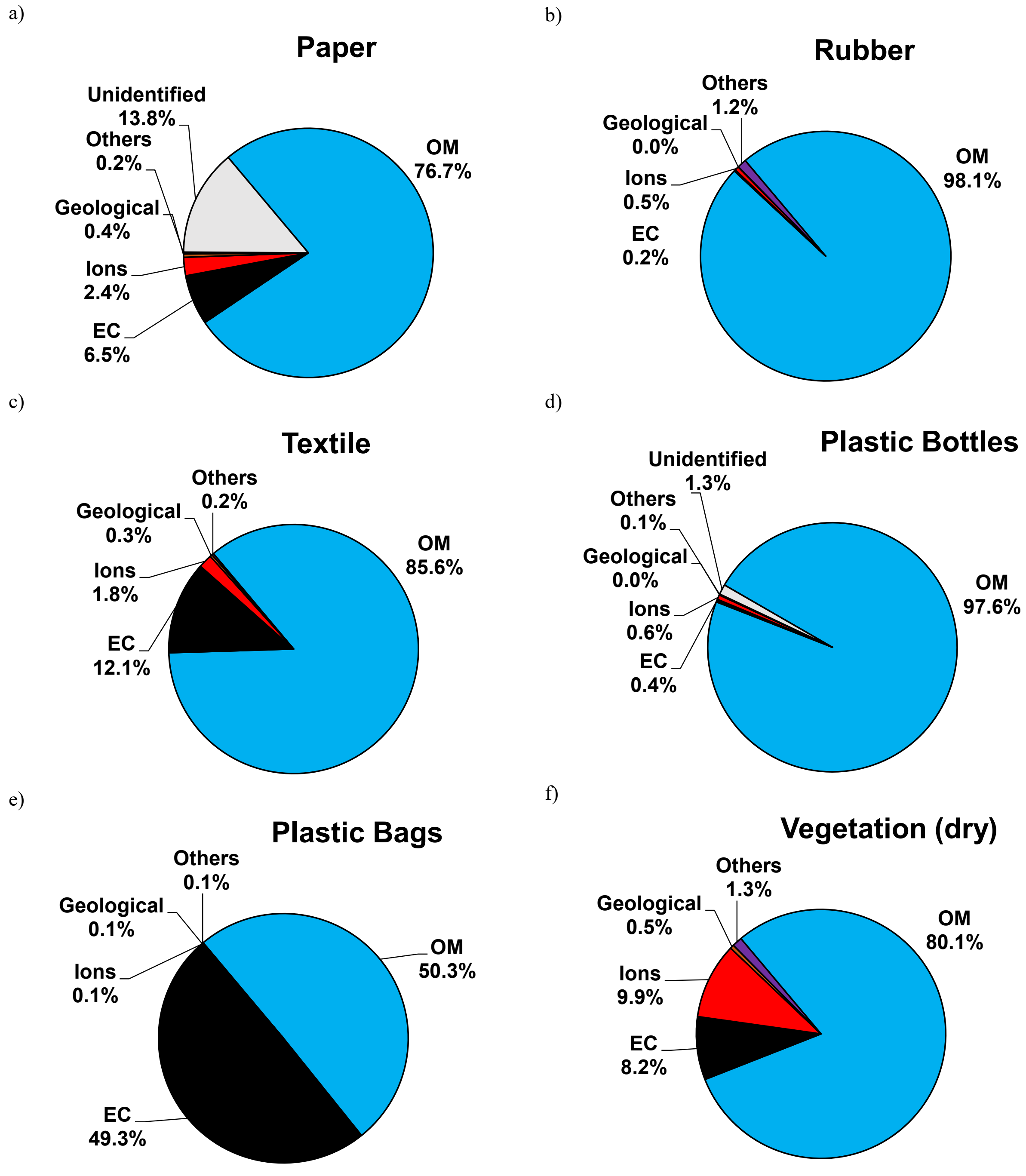


Figure S2: Major chemical composition (% of $PM_{2.5}$ mass) for waste materials tested.

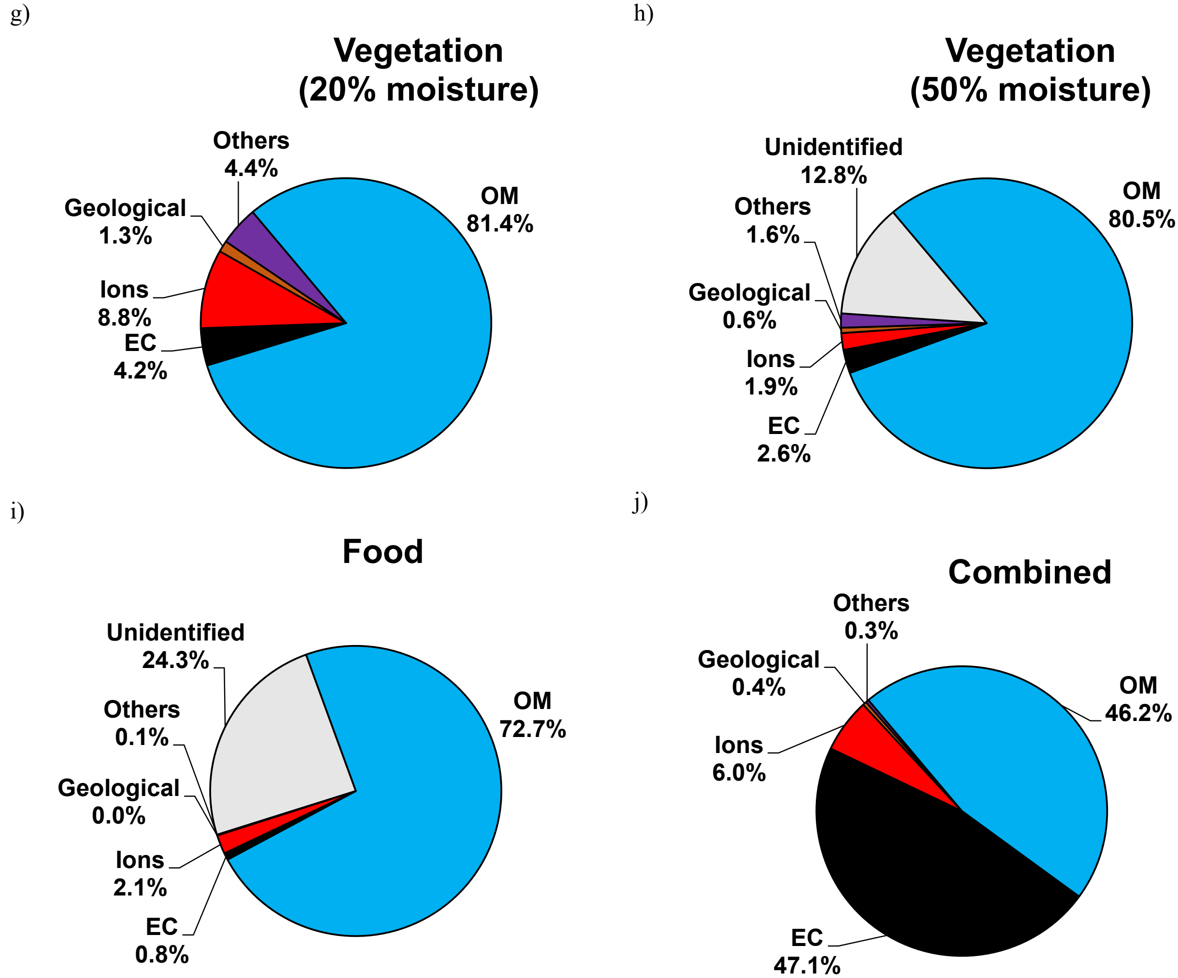


Figure S2 continued.

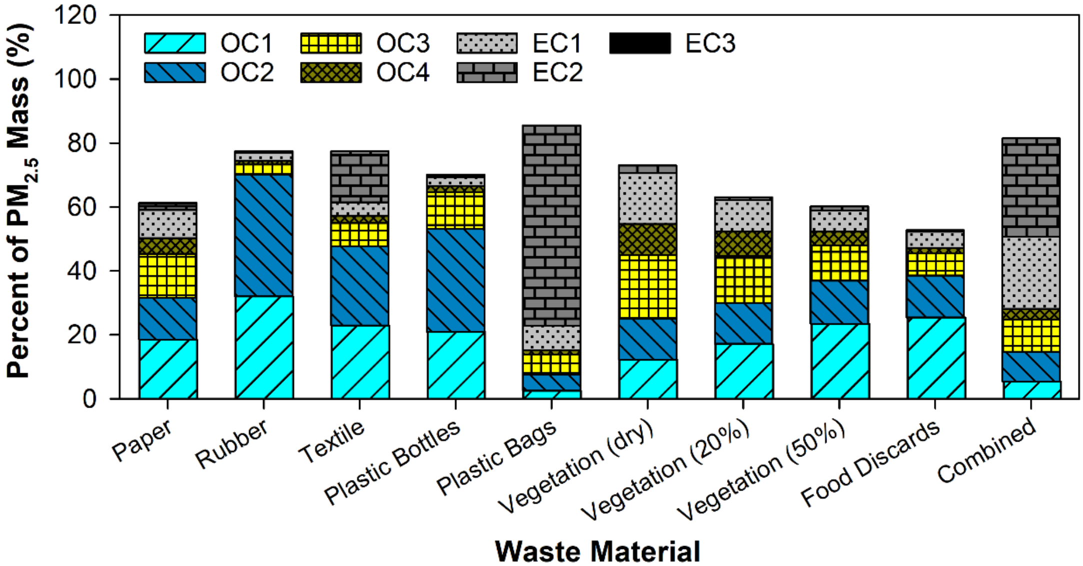
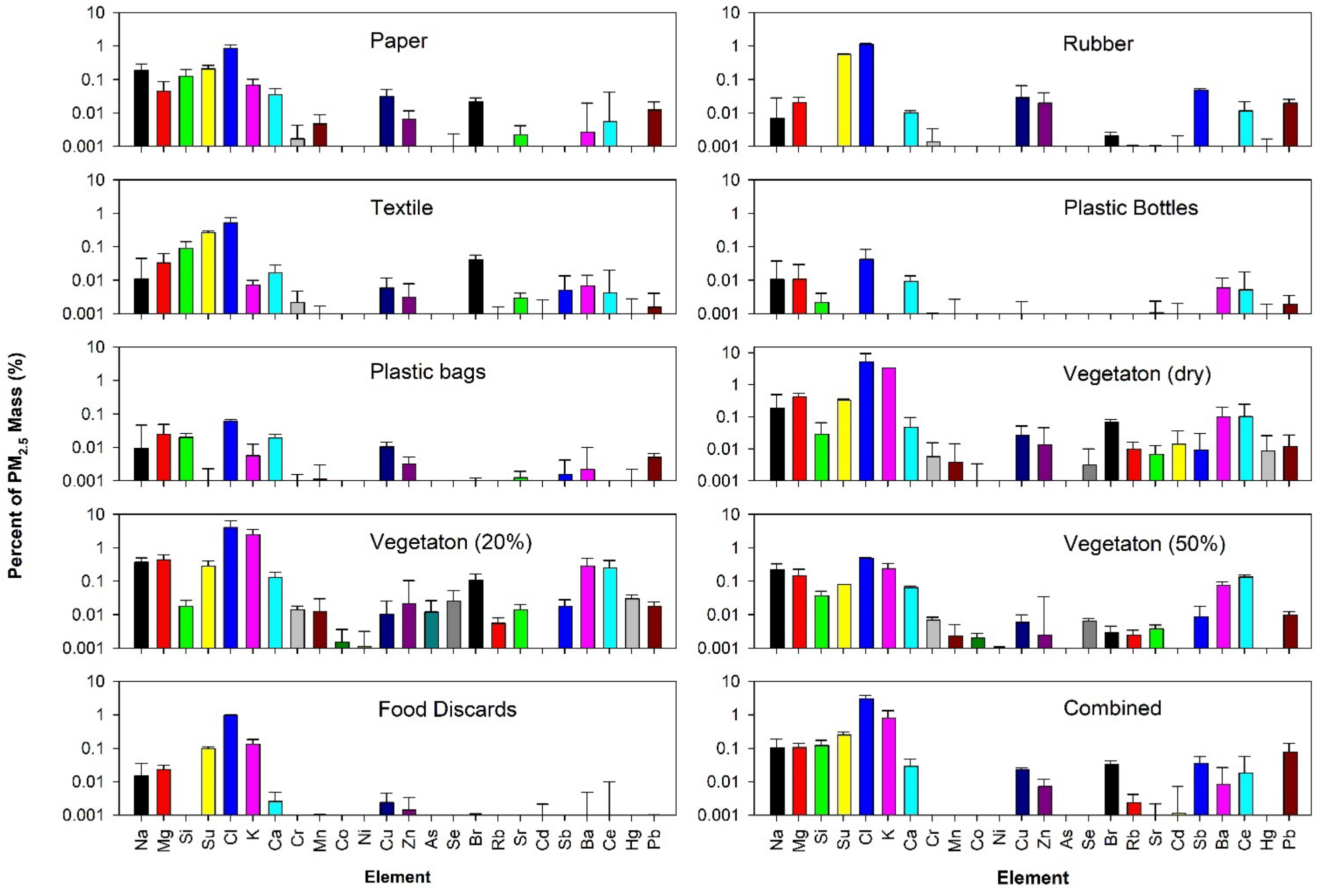


Figure S3: Abundances of carbon fractions (% of $PM_{2.5}$ mass).



60 **Figure S4: Abundances of elements (% of $PM_{2.5}$ mass).**

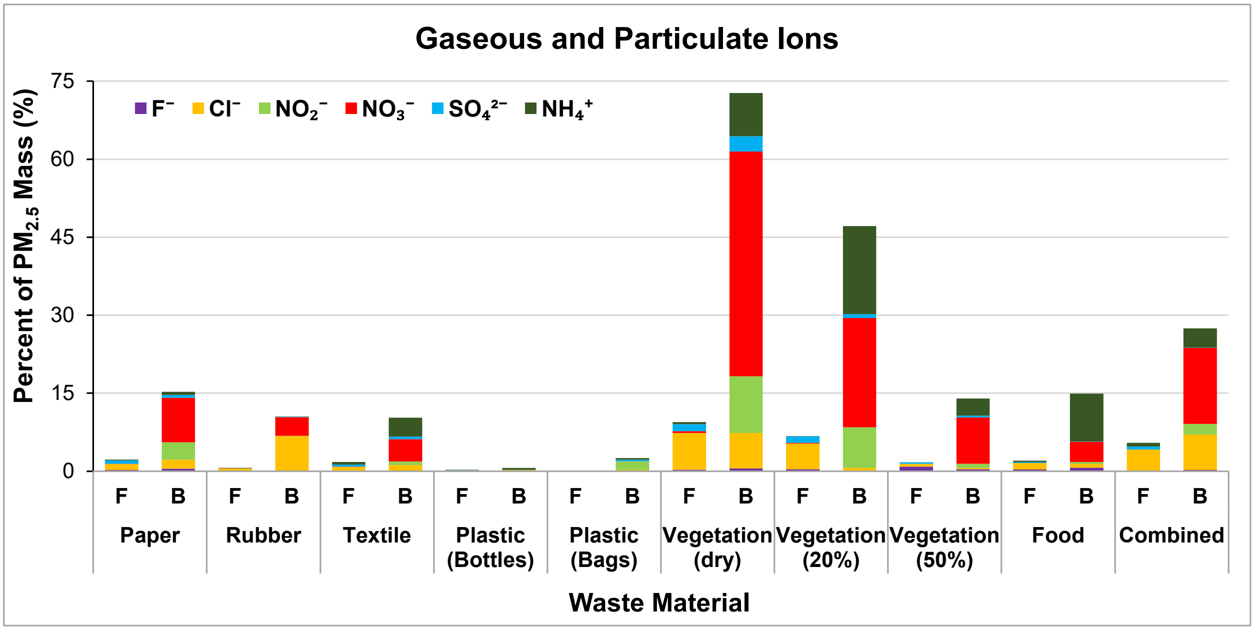


Figure S5: Abundances of particulate ions captured on the front (F) quartz-fiber filters and gaseous ions collected on the back (B) impregnated filters (see filter configuration in Figure 1). The sum of the particulate inorganic ions on the front filters was less than 10% of $PM_{2.5}$ mass for all waste materials. Among the three vegetations, particulate ions were most abundant in dry vegetation (9.9%), and their abundances decreased with increasing moisture content, likely due to lower combustion temperatures decreasing the generation of these ions. The gaseous ions were more abundant than particulate ions and the dry vegetation had higher gaseous ion than those with higher moisture content. The vegetation samples show high abundances of HCl, HNO_2, HNO_3, and NH_3. The rubber sample had a higher HCl abundance (6.7%) than for the other samples except for dry vegetation.

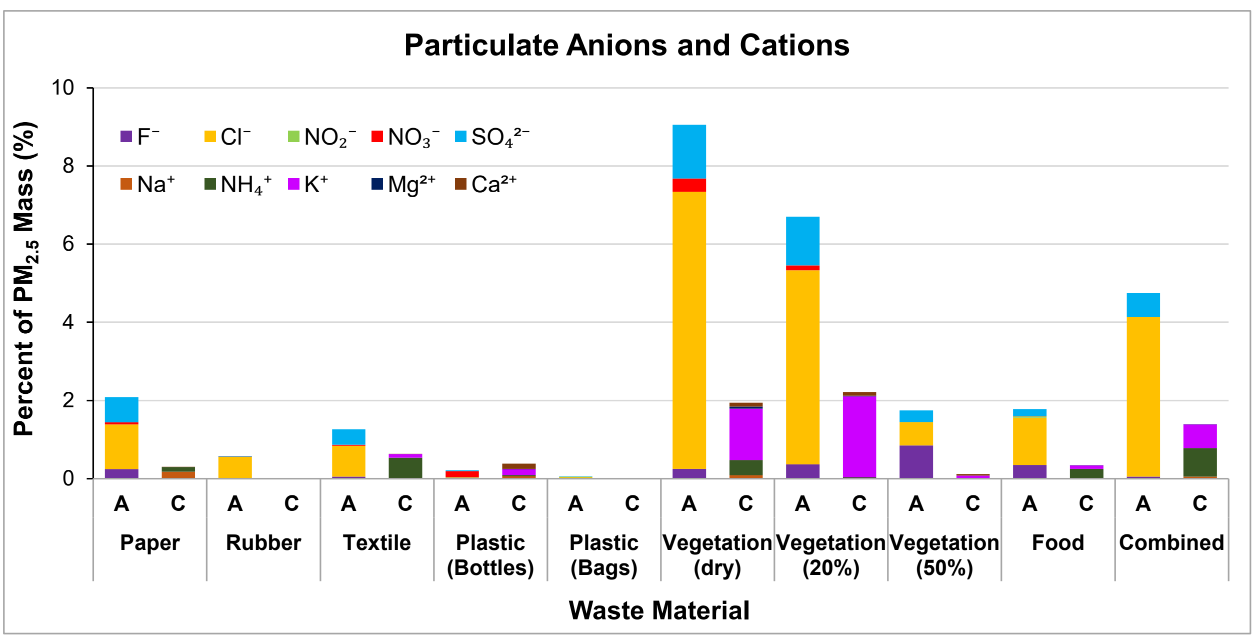
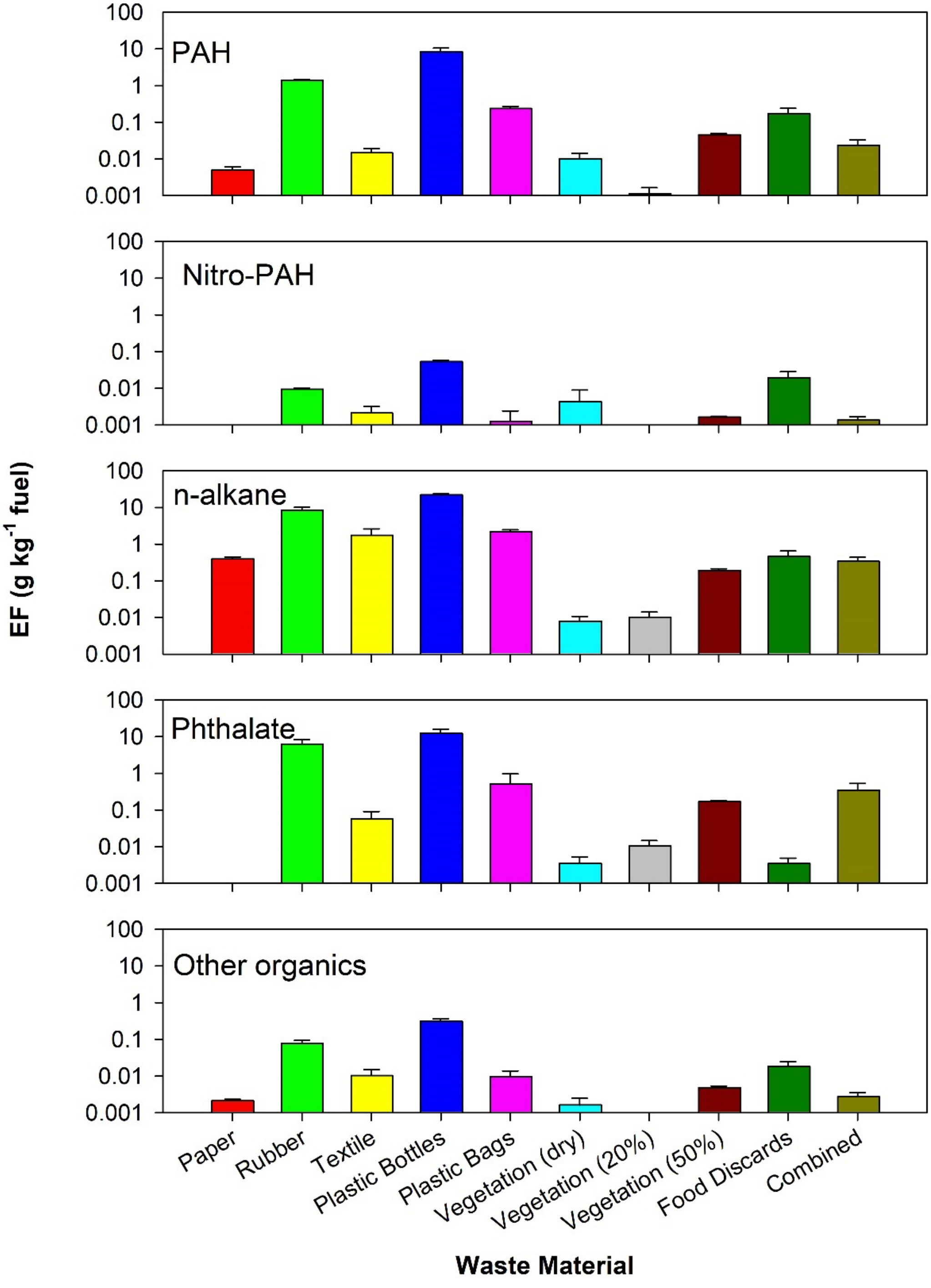


Figure S6: Abundances of particulate anion (A) and cation (C) captured on the front quartz-fiber filters (% of $PM_{2.5}$ mass).



75 **Figure S7: Emission factors of organic species.**

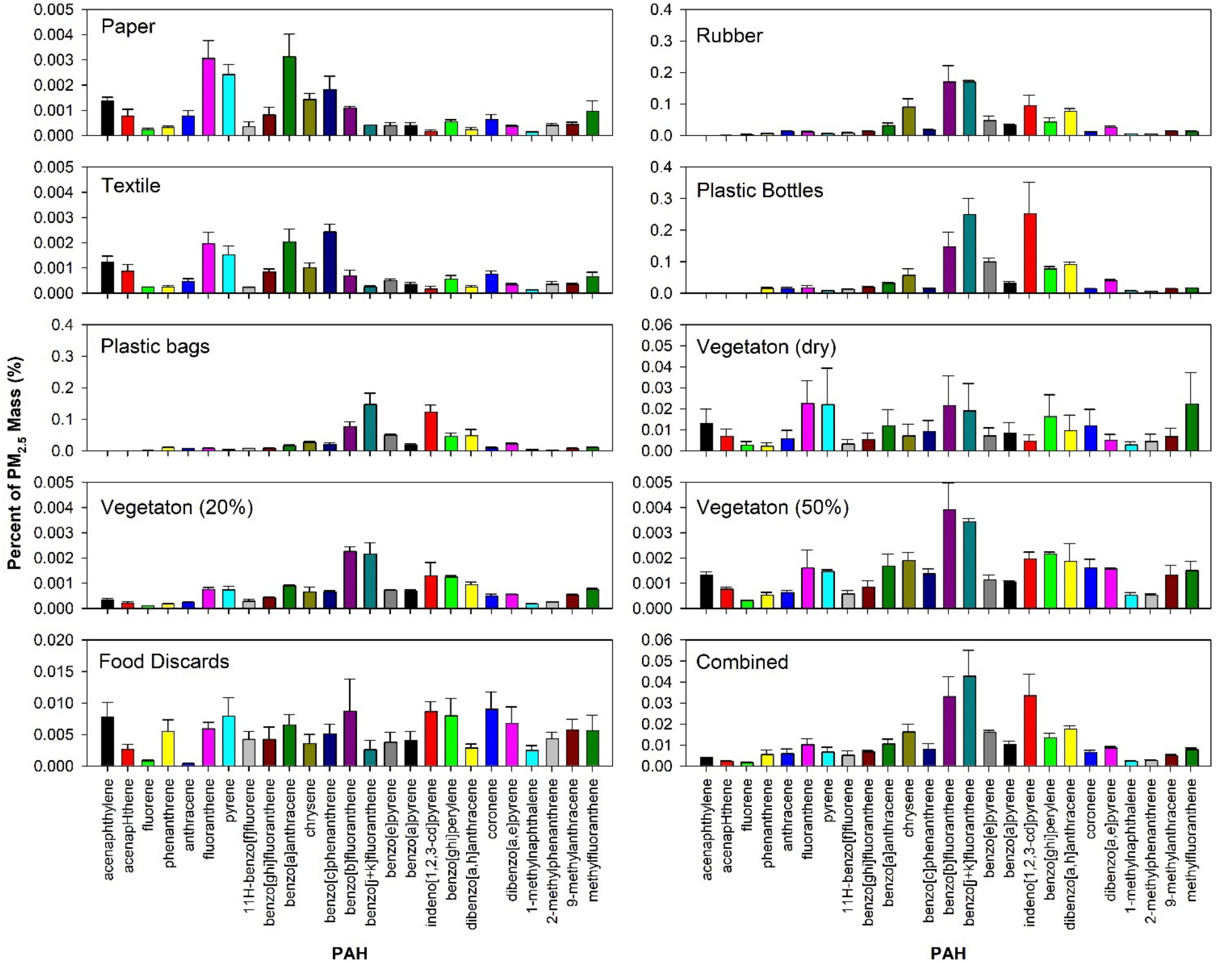


Figure S8: Abundances of PAHs (% of $PM_{2.5}$ mass).

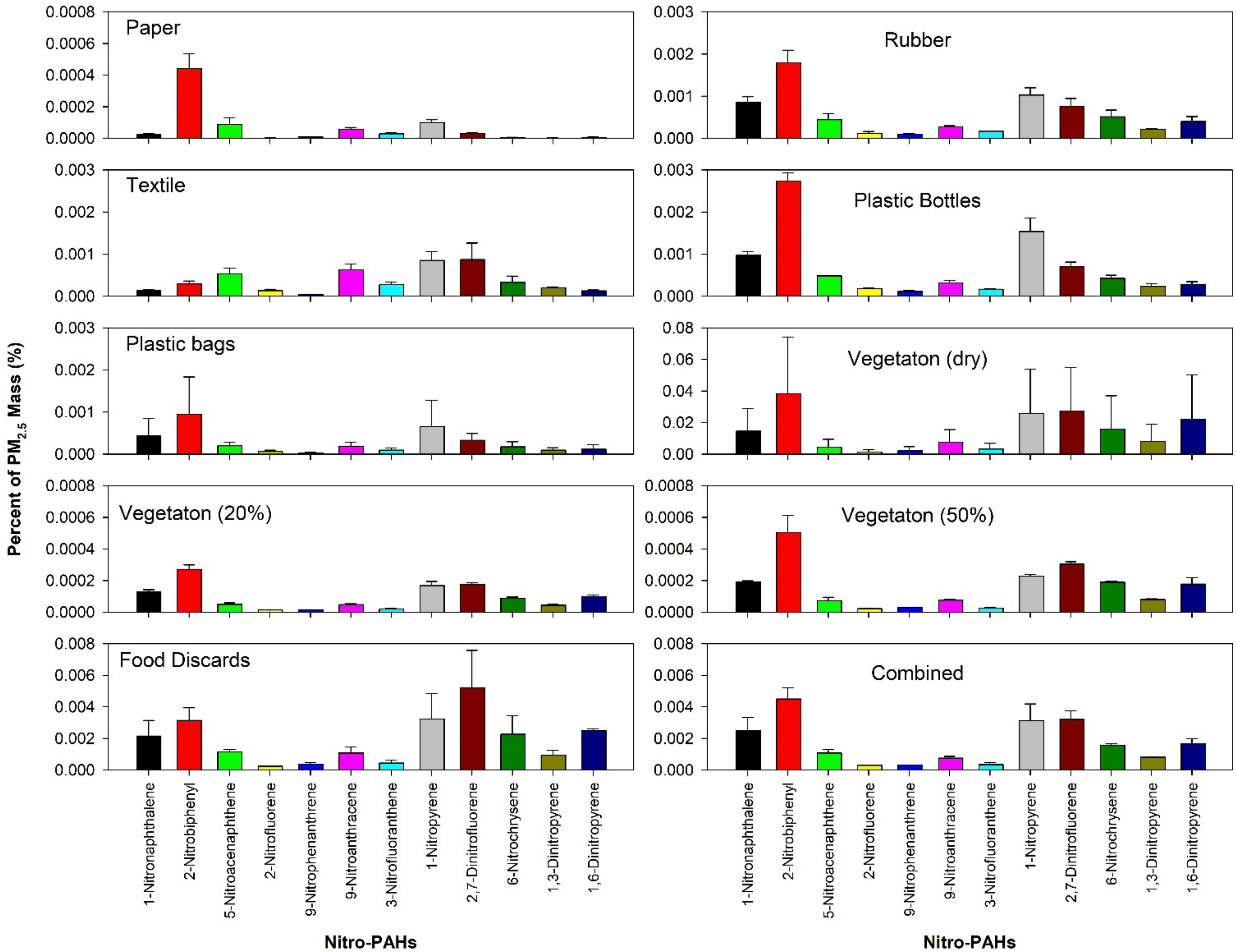


Figure S9: Abundances of nitro-PAHs (% of $PM_{2.5}$ mass).

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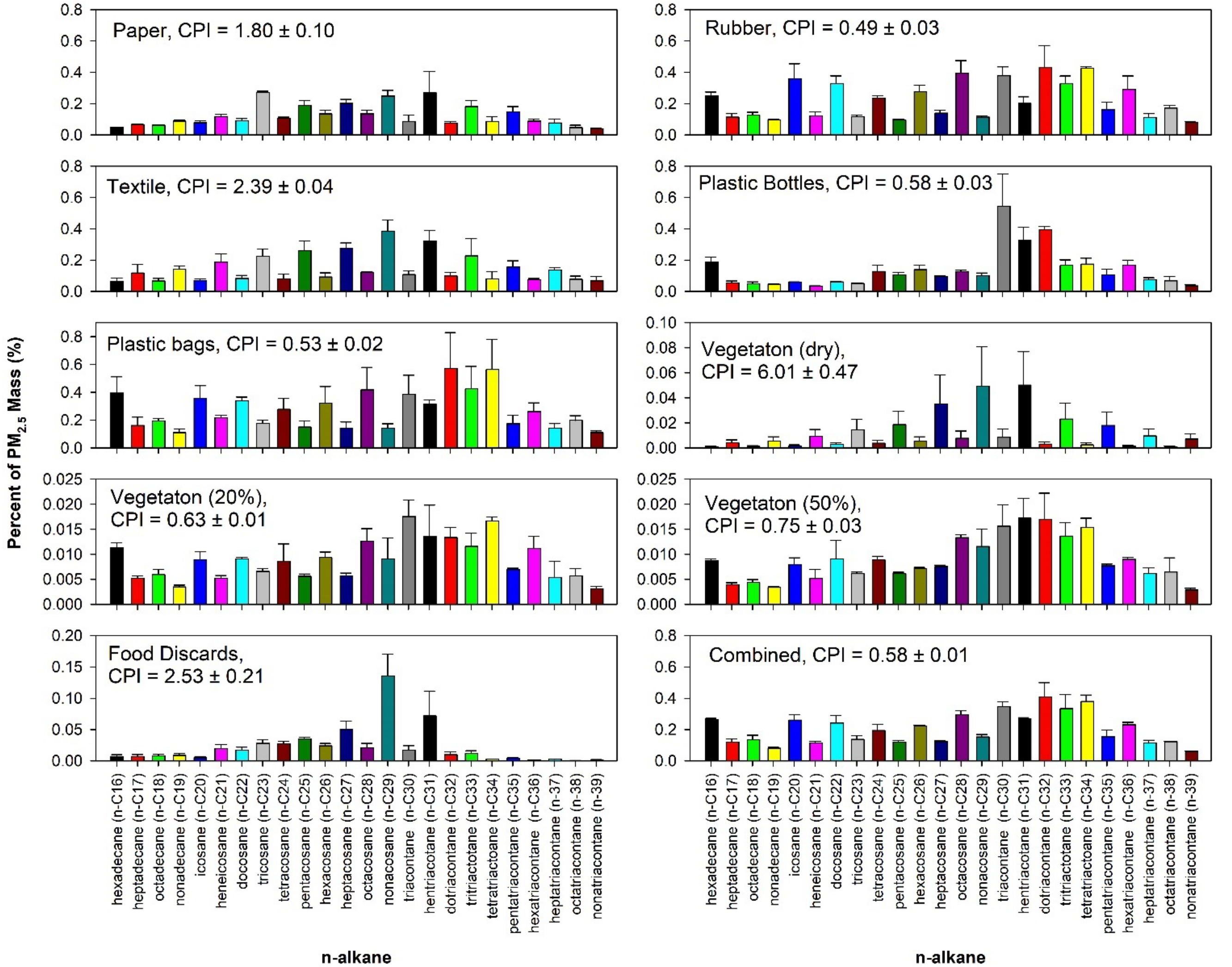
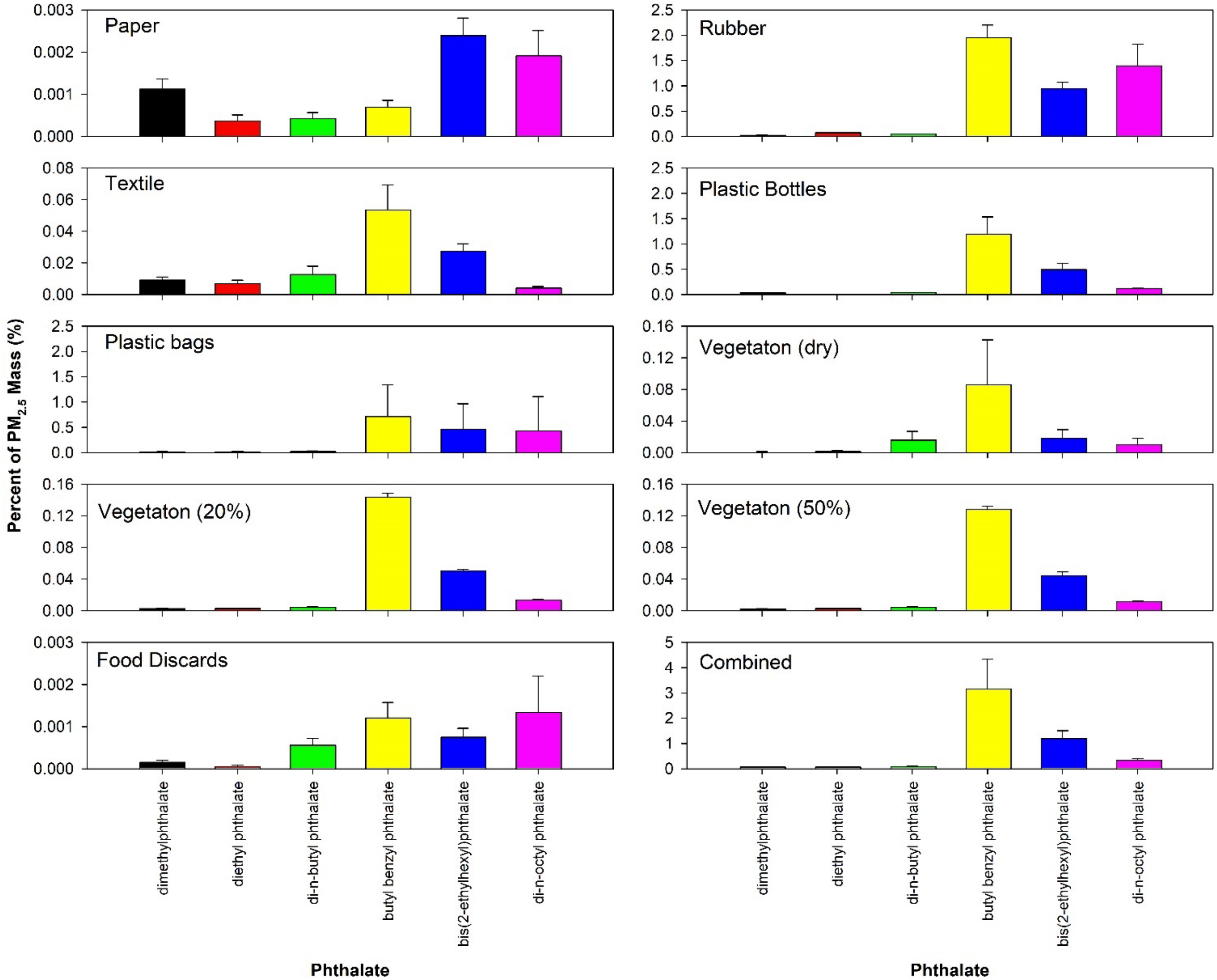


Figure S10: Abundances of n-alkanes (% of $PM_{2.5}$ mass).



85 **Figure S11: Abundances of phthalates (% of $PM_{2.5}$ mass).**

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