

Supplemental information for:

“Positive matrix factorization of $PM_{2.5}$ – Eliminating the effects of gas/particle partitioning of semivolatile organic compounds”

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Table S1.

Statistics for the total concentration of each SVOC estimated from January 27, 2003 – October 2, 2005 (Full data set).

	Abbreviation	Mean	Median	Mean fraction (%) ^a	S/N ^b	CV ^c	$p^{\circ}L$ (atm, 298K) ^d	ΔH_{vap} (kJ mol ⁻¹ , 298K) ^e	$K_{p,om}$ (m ³ μg^{-1}) ^f
Bulk species ($\mu\text{g m}^{-3}$) ^g									
Mass*		8.05	7.03		3.89	0.61			
Nitrate	Nitr	1.00	0.22		6.53	1.73			
Sulfate	Sulf	1.18	0.97		13.3	0.88			
Ammonium*	Ammo	0.56	0.43		14.2	1.04			
EC		0.51	0.43		6.53	0.69			
OC1*		1.28	1.20		4.58	0.43			
OC2		0.65	0.59		4.32	0.50			
OC3		0.43	0.41		2.39	0.43			
OC4*		0.03	0.01		1.00	2.30			
PC		0.38	0.28		2.46	0.94			
Organic molecular makers (ng m ⁻³)									
<i>Alkanes</i>									
docosane	C22	32.8	15.1	16.1	1.46	2.48	3.2E-08	115	8.73E-02
tricosane	C23	23.7	7.40	28.6	1.60	2.38	1.2E-08	120	2.76E-01
tetracosane	C24	5.50	2.27	44.3	1.63	1.83	4.6E-09	124	8.72E-01
pentacosane	C25	3.73	2.02	61.3	1.36	2.21	1.7E-09	129	2.77E+00
hexacosane	C26	1.14	0.94	76.9	0.77	2.14	6.5E-10	133	8.83E+00
heptacosane	C27	1.27	1.09	88.3	0.67	2.48	2.5E-10	137	2.82E+01
octacosane	C28	0.79	0.54	94.8	0.93	2.28	9.3E-11	142	9.05E+01
nonacosane	C29	1.72	1.40	97.9	0.77	2.37	3.5E-11	146	2.91E+02
triacontane	C30	0.64	0.39	99.2	1.04	1.89	1.3E-11	151	9.39E+02
hentriacontane	C31	1.78	1.30	99.7	1.17	1.10	4.9E-12	155	3.04E+03
dotriacontane*	C32	0.51	0.23	99.9	1.61	0.70	1.9E-12	160	9.86E+03
trtriacontane	C33	0.62	0.47	100	0.88	1.95	7.0E-13	164	3.21E+04
tetratriacontane	C34	0.45	0.31	100	1.01	2.01	2.6E-13	169	1.05E+05
pentatriacontane	C35	0.38	0.27	100	0.96	2.02	9.9E-14	173	3.42E+05
hexatriacontane	C36	0.20	0.12	100	1.19	1.75	3.7E-14	177	1.12E+06
heptatriacontane	C37	0.16	0.08	100	1.30	1.54	1.4E-14	182	3.69E+06
octatriacontane	C38	0.13	0.05	100	1.32	1.36	5.3E-15	186	1.22E+07
nonatriacontane*	C39	0.12	0.06	100	1.23	1.32	2.0E-15	191	4.02E+07
tetracontane*	C40	0.09	0.04	100	1.29	1.14	7.5E-16	195	1.33E+08
pentadecylcyclohexane	cycC21	8.07	3.62	7.30	1.67	2.01	8.2E-08	107	2.50E-02
nonadecylcyclohexane*	cycC25	0.26	0.21	61.3	0.77	1.86	1.6E-09	124	2.47E+00
<i>PAHs</i>									
fluoranthene	Flu	11.2	7.33	4.12	1.16	1.74	1.1E-07	92.2	1.14E-02
pyrene	Pyr	1.48	1.08	14.7	1.04	1.78	2.4E-08	98.9	6.40E-02
benzo[ghi]fluoranthene	BghiF	0.19	0.15	44.3	0.74	2.16	3.3E-09	104	5.64E-01
cyclopenta[cd]pyrene	C-pyr	0.06	0.03	48.5	1.38	2.10	2.5E-09	103	6.94E-01
benz[a]anthracene	BaA	0.12	0.08	44.6	1.16	2.12	3.4E-09	108	6.24E-01
chrysene/triphenylene*	CT	0.48	0.38	44.6	1.06	2.65	3.4E-09	108	6.24E-01
benzo[b&k]fluoranthene	BbkF	0.27	0.16	79.3	1.15	2.18	4.6E-10	113	5.54E+00
benzo[j]fluoranthene*	BjF	0.01	0.01	79.3	3.62	0.91	4.6E-10	113	5.54E+00
benz[a&e]pyrene	BaeP	0.20	0.09	93.7	1.35	2.25	1.0E-10	119	3.18E+01
perylene*	Per	0.02	0.01	93.7	1.66	1.28	1.0E-10	119	3.18E+01
indeno[1,2,3-cd]pyrene	IP	0.07	0.04	99.1	1.17	2.42	1.4E-11	124	2.85E+02
benzo[ghi]perylene	BP	0.18	0.11	99.8	1.14	2.60	3.2E-12	132	1.65E+03
dibenz[ah]anthracene*	DahA	0.02	0.01	99.0	1.47	1.76	1.5E-11	128	3.19E+02
picene*	Pic	0.02	0.01	99.0	3.70	1.45	1.5E-11	128	3.19E+02
coronene	Cor	0.11	0.06	100	1.27	1.53	9.7E-14	142	8.79E+04
methyl-202-PAH sum	M-202	8.70	6.67	9.90	0.93	1.70	4.0E-08	96.6	3.54E-02
retene*	Ret	1.98	1.17	20.9	1.40	1.54	1.6E-08	105	1.22E-01
methyl-228-PAH sum	M-228	0.19	0.13	63.0	0.99	2.26	1.3E-09	112	1.96E+00

^a mean fraction of particle-phase SVOC; ^b signal to noise ratio = mean concentration/mean uncertainty; ^c coefficient of variation = standard deviation/mean concentration; ^d pure compound vapor pressure at 298.15 K; ^e enthalpy of vaporization of the liquid; ^f average value; ^g obtained from filter measurement, not including gas phase; * species not included for PMF analysis.

Table S1. Continued

	Abbreviation	Mean	Median	Mean fraction (%)	S/N	CV	$p^{\circ}L$ (atm) @ 298K	ΔH_{vap} (kJ mol ⁻¹) @ 298K	$K_{p, \text{om}}$ (m ³ μg ⁻¹)
<i>Oxy-PAHs</i>									
acenaphthenone*	Ace-O	440	146	0.09	2.15	0.73	2.9E-06	71.4	2.17E-04
fluorenone*	Flu-O	467	226	0.29	2.23	0.88	1.1E-06	75.8	6.61E-04
1H-phenalen-1-one*	Phe-O	303	145	0.35	1.65	1.48	8.4E-07	74.7	8.19E-04
xanthone*	Xan	44.9	26.2	1.52	1.17	2.03	2.3E-07	81.8	3.70E-03
1,8-naphthalic anhydride	Nap-DO	64.7	41.7	1.61	1.11	2.00	1.9E-07	76.9	3.92E-03
anthracene-9,10-dione	Ant-DO	21.1	11.4	6.04	1.25	2.01	4.7E-08	79.9	1.73E-02
benz[de]anthracene-7-one	BaA-O	0.22	0.18	35.8	0.71	2.43	4.7E-09	96.2	3.02E-01
<i>Steranes</i>									
20R-abb & 20S-aaa-cholestane	27-RS-C	0.19	0.15	89.3	0.93	2.44	2.0E-10	121	1.77E+01
20R & S-abb-methylcholestane	28-RS-M	0.13	0.08	95.4	1.25	2.47	7.5E-11	125	5.59E+01
20R & S-abb-ethylcholestane	29-RS-E	0.14	0.09	98.2	1.13	2.62	2.8E-11	130	1.78E+02
a-22,29,30-trisnorhopane	TS	0.11	0.09	89.5	0.84	2.64	1.9E-10	117	1.58E+01
ba-30-norhopane	ba-N	0.38	0.25	98.3	1.16	2.50	2.7E-11	126	1.58E+02
ab-hopane	ab-H	0.27	0.16	99.3	1.30	2.42	1.0E-11	130	5.03E+02
22S-ab-30-homohopane	31abS	0.12	0.07	99.8	1.31	2.45	3.8E-12	134	1.61E+03
22R-ab-30-homohopane	31abR	0.09	0.05	99.8	1.30	2.39	3.8E-12	134	1.61E+03
22S-ab-30-bishomohopane	32abS	0.07	0.05	99.9	1.24	2.37	1.4E-12	139	5.14E+03
22R-ab-30-bishomohopane	32abR	0.06	0.04	99.9	1.16	2.31	1.4E-12	139	5.14E+03
<i>Alkanoic acids</i>									
dodecanoic acid	C12:0	710	336	2.81	1.63	1.70	1.8E-07	93.6	7.36E-03
tridecanoic acid*	C13:0	30.9	6.76	7.08	1.89	0.86	6.6E-08	98.1	2.29E-02
tetradecanoic acid*	C14:0	160	60.5	15.4	1.60	1.86	2.5E-08	103	7.12E-02
pentadecanoic acid*	C15:0	14.0	5.57	28.5	1.63	1.43	9.3E-09	107	2.23E-01
hexadecanoic acid	C16:0	90.6	44.6	45.3	1.44	1.60	3.5E-09	111	6.98E-01
heptadecanoic acid*	C17:0	2.18	1.35	63.3	1.33	0.71	1.3E-09	116	2.20E+00
octadecanoic acid	C18:0	17.6	11.5	79.2	1.13	1.55	5.0E-10	120	6.94E+00
oleic acid*	C18:1	2.59	0.18	82.3	2.67	1.91	3.9E-10	119	8.51E+00
<i>Sterols and methoxyphenols</i>									
cholesterol*	Cho	0.39	0.17	99.9	1.51	1.13	1.0E-12	136	6.52E+03
stigmasterol*	Sti	0.49	0.22	100	1.43	1.35	1.1E-13	144	8.20E+04
vanillin*	Van	271	163	1.58	1.43	1.28	2.2E-07	80.7	3.84E-03
acetovanillone*	Acv	67.3	32.1	1.45	1.42	0.83	2.0E-07	74.7	3.51E-03
coniferaldehyde*	Con	11.7	5.55	12.3	1.66	1.44	2.4E-08	88.4	4.50E-02
syringaldehyde*	Syr	5.55	2.64	26.1	2.13	1.43	8.0E-09	92.0	1.53E-01
acetosyringone*	Ace	1.88	0.46	25.6	1.79	0.78	7.2E-09	86.0	1.38E-01

Table S2.

Statistics for the total concentration of each SVOC estimated for sampling days with ambient temperature lower than 10 °C (Cold period).

	Abbreviation	Mean	Median	Mean fraction (%)	CV	S/N	$K_{p,om}$ ($m^3 \mu g^{-1}$)
Bulk species ($\mu g m^{-3}$)							
Mass*		9.57	7.64		0.70	4.13	
Nitrate	Nitr	2.23	1.41		1.04	12.2	
Sulfate	Sulf	1.30	0.79		1.13	13.5	
Ammonium*	Ammo	0.88	0.56		1.02	21.0	
EC		0.61	0.48		0.75	7.20	
OC1*		1.29	1.13		0.55	4.64	
OC2		0.56	0.48		0.54	4.61	
OC3		0.40	0.35		0.53	2.51	
OC4*		0.04	0.01		2.27	1.00	
PC		0.42	0.30		1.03	2.60	
Organic molecular makers (ng m ⁻³)							
<i>Alkanes</i>							
docosane	C22	6.31	4.89	35.5	2.75	0.82	2.12E-01
tricosane	C23	3.11	2.54	57.8	2.45	0.69	6.76E-01
tetracosane	C24	1.56	1.43	77.7	1.53	0.54	2.16E+00
pentacosane	C25	1.59	1.39	90.4	2.35	0.60	6.92E+00
hexacosane	C26	1.22	1.07	96.4	2.50	0.66	2.22E+01
heptacosane	C27	1.37	1.19	98.7	2.60	0.69	7.15E+01
octacosane	C28	1.17	1.00	99.6	2.72	0.73	2.31E+02
nonacosane	C29	1.41	1.21	99.9	2.62	0.70	7.46E+02
triacontane	C30	0.98	0.89	100	2.25	0.78	2.42E+03
hentriacontane	C31	1.43	1.23	100	2.13	0.76	7.86E+03
dotriacontane*	C32	0.49	0.32	100	1.09	1.14	2.56E+04
tritriacontane	C33	0.73	0.55	100	2.04	0.90	8.36E+04
tetracontane	C34	0.58	0.43	100	2.12	0.91	2.73E+05
pentatriacontane	C35	0.55	0.42	100	2.22	0.85	8.97E+05
hexatriacontane	C36	0.32	0.22	100	2.01	0.96	2.95E+06
heptatriacontane	C37	0.27	0.18	100	1.85	0.99	9.72E+06
octatriacontane	C38	0.22	0.15	100	1.68	0.99	3.21E+07
nonatriacontane	C39	0.20	0.14	100	1.60	0.96	1.06E+08
tetracontane*	C40	0.15	0.10	100	1.40	1.00	3.52E+08
pentadecylcyclohexane	cycC21	1.93	1.30	16.7	1.92	1.06	5.93E-02
nonadecylcyclohexane*	cycC25	0.22	0.18	89.9	1.98	0.71	6.11E+00
<i>PAHs</i>							
fluoranthene	Flu	4.15	3.08	9.18	1.69	0.84	2.58E-02
pyrene	Pyr	0.81	0.70	31.1	1.84	0.72	1.48E-01
benzo[ghi]fluoranthene	BghiF	0.22	0.19	73.7	2.38	0.67	1.33E+00
cyclopenta[cd]pyrene	C-pyr	0.09	0.06	77.2	2.61	1.03	1.63E+00
benz[a]anthracene	BaA	0.15	0.11	74.9	2.58	0.89	1.48E+00
chrysene/triphenylene*	CT	0.42	0.33	74.9	2.86	0.74	1.48E+00
benzo[b&k]fluoranthene	BbkF	0.42	0.31	95.6	2.42	0.78	1.34E+01
benzo[j]fluoranthene*	BjF	0.02	0.01	95.6	1.44	3.53	1.34E+01
benz[a&e]pyrene	BaeP	0.36	0.24	99.1	2.47	0.93	7.79E+01
perylene*	Per	0.03	0.02	99.1	1.62	1.19	7.79E+01
indeno[1,2,3-cd]pyrene	IP	0.13	0.11	99.9	2.58	0.76	7.05E+02
benzo[ghi]perylene	BP	0.32	0.25	100	2.85	0.80	4.15E+03
dibenz[ah]anthracene*	DahA	0.04	0.03	99.9	2.25	0.92	7.97E+02
picene*	Pic	0.03	0.02	99.9	2.05	0.95	7.97E+02
coronene	Cor	0.18	0.13	100	1.50	0.91	2.24E+05
methyl-202-PAH sum	M-202	5.85	4.89	21.5	1.80	0.71	8.13E-02
retene*	Ret	2.44	1.74	43.1	1.81	1.22	2.87E-01
methyl-228-PAH sum	M-228	0.26	0.18	89.0	2.49	0.91	4.72E+00

* Species not included for PMF analysis.

Table S2. Continued

	Abbreviation	Mean	Median	Mean fraction (%)	CV	S/N	$K_{p,om}$ ($m^3 \mu g^{-1}$)
<i>Oxy-PAHs</i>							
acenaphthenone*	Ace-O	463	176	0.20	1.18	2.88	4.42E-04
fluorenone*	Flu-O	455	162	0.61	1.16	3.25	1.38E-03
1H-phenalen-1-one*	Phe-O	204	89.8	0.75	1.11	1.82	1.70E-03
xanthone*	Xan	9.07	7.31	3.31	1.98	0.87	7.98E-03
1,8-naphthalic anhydride	Nap-DO	15.9	12.8	3.41	2.00	0.70	8.23E-03
anthracene-9,10-dione	Ant-DO	4.53	3.54	12.6	2.00	0.76	3.68E-02
benz[de]anthracene-7-one	BaA-O	0.23	0.19	62.9	2.77	0.63	6.92E-01
<i>Steranes</i>							
20R-abb & 20S-aaa-cholestane	27-RS-C	0.24	0.15	98.4	2.62	1.07	4.34E+01
20R & S-abb-methylcholestane	28-RS-M	0.20	0.11	99.5	2.42	1.18	1.39E+02
20R & S-abb-ethylcholestane	29-RS-E	0.22	0.14	99.8	2.92	1.02	4.45E+02
a-22,29,30-trisnorhopane	TS	0.13	0.09	98.3	2.96	0.97	3.85E+01
ba-30-norhopane	ba-N	0.59	0.37	99.8	2.68	1.07	3.93E+02
ab-hopane	ab-H	0.43	0.27	99.9	2.63	1.12	1.26E+03
22S-ab-30-homohopane	31abS	0.19	0.12	100	2.66	1.11	4.05E+03
22R-ab-30-homohopane	31abR	0.14	0.09	100	2.65	1.12	4.05E+03
22S-ab-30-bishomohopane	32abS	0.11	0.07	100	2.64	1.12	1.30E+04
22R-ab-30-bishomohopane	32abR	0.09	0.05	100	2.60	1.05	1.30E+04
<i>Alkanoic acids</i>							
dodecanoic acid	C12:0	108	63.8	6.35	1.97	1.32	1.67E-02
tridecanoic acid*	C13:0	4.06	1.42	15.8	0.77	1.90	5.27E-02
tetradecanoic acid*	C14:0	19.0	11.5	32.8	1.50	1.14	1.67E-01
pentadecanoic acid*	C15:0	2.33	1.66	55.4	1.38	0.89	5.28E-01
hexadecanoic acid	C16:0	34.0	25.1	76.2	1.96	0.93	1.68E+00
heptadecanoic acid*	C17:0	1.18	0.74	89.7	1.04	1.00	5.34E+00
octadecanoic acid	C18:0	15.5	10.5	96.1	1.74	0.96	1.70E+01
oleic acid*	C18:1	5.39	0.60	96.8	2.33	1.87	2.09E+01
<i>Sterols and methoxyphenols</i>							
cholesterol*	Cho	0.60	0.28	100	1.46	1.37	1.65E+04
stigmasterol*	Sti	0.77	0.49	100	2.27	1.13	2.10E+05
vanillin*	Van	328	224	3.41	1.51	1.13	8.23E-03
acetovanillone*	Acv	76.0	55.7	3.04	1.04	0.95	7.28E-03
coniferaldehyde*	Con	15.9	10.1	25.3	1.79	1.21	9.98E-02
syringaldehyde*	Syr	7.95	5.05	49.0	1.75	1.28	3.45E-01
acetosyringone*	Ace	1.98	1.19	47.1	1.80	1.20	3.03E-01

Table S3.

Statistics for the total concentration of each SVOC estimated for sampling days with ambient temperature between 10 °C and 20 °C (Warm period).

	Abbreviation	Mean	Median	Mean fraction (%)	CV	S/N	$K_{p, om}$ ($m^3 \mu g^{-1}$)
Bulk species ($\mu g m^{-3}$)							
Mass*		6.54	6.18		0.44	3.26	
Nitrate	Nitr	0.37	0.17		1.58	2.56	
Sulfate	Sulf	1.01	0.90		0.67	12.4	
Ammonium*	Ammo	0.32	0.23		0.96	14.0	
EC		0.43	0.36		0.62	6.35	
OC1*		1.08	1.05		0.33	4.67	
OC2		0.57	0.54		0.46	4.76	
OC3		0.39	0.38		0.38	2.64	
OC4*		0.03	0.01		2.23	1.00	
PC		0.28	0.22		0.78	2.57	
Organic molecular makers (ng m ⁻³)							
<i>Alkanes</i>							
docosane	C22	23.2	18.0	6.42	2.40	0.84	1.97E-02
tricosane	C23	12.2	8.53	15.9	2.33	0.91	5.62E-02
tetracosane	C24	2.56	2.15	33.7	1.41	0.80	1.60E-01
pentacosane	C25	1.86	1.63	57.1	2.07	0.66	4.56E-01
hexacosane	C26	0.81	0.61	77.8	1.94	0.86	1.30E+00
heptacosane	C27	0.98	0.84	90.3	2.25	0.70	3.71E+00
octacosane	C28	0.61	0.36	96.2	1.94	0.99	1.06E+01
nonacosane	C29	1.49	1.19	98.6	2.22	0.75	3.02E+01
triacontane	C30	0.49	0.27	99.5	1.59	1.07	8.61E+01
hentriacontane	C31	1.50	1.09	99.8	1.19	0.88	2.46E+02
dotriacontane*	C32	0.39	0.21	99.9	0.65	1.66	7.02E+02
tritriacontane	C33	0.51	0.41	100	1.84	0.84	2.00E+03
tetratriacontane	C34	0.37	0.28	100	1.84	0.98	5.73E+03
pentatriacontane	C35	0.28	0.23	100	1.76	0.86	1.64E+04
hexatriacontane	C36	0.14	0.09	100	1.48	1.09	4.68E+04
heptatriacontane	C37	0.11	0.05	100	1.27	1.22	1.34E+05
octatriacontane	C38	0.09	0.04	100	1.12	1.19	3.82E+05
nonatriacontane	C39	0.09	0.05	100	1.12	1.16	1.09E+06
tetracontane*	C40	0.06	0.04	100	0.96	1.16	3.13E+06
pentadecylcyclohexane	cycC21	7.11	4.84	2.36	1.99	1.00	6.85E-03
nonadecylcyclohexane*	cycC25	0.18	0.16	57.0	1.83	0.65	4.50E-01
<i>PAHs</i>							
fluoranthene	Flu	10.8	8.22	1.46	1.73	0.95	4.18E-03
pyrene	Pyr	1.32	1.05	6.70	1.76	0.79	2.05E-02
benzo[ghi]fluoranthene	BghiF	0.16	0.13	34.8	2.12	0.70	1.64E-01
cyclopenta[cd]pyrene	C-pyr	0.04	0.03	39.9	1.89	1.20	2.07E-01
benz[a]anthracene	BaA	0.09	0.05	34.9	2.05	1.17	1.66E-01
chrysene/triphenylene*	CT	0.39	0.33	34.9	2.50	0.67	1.66E-01
benzo[b&k]fluoranthene	BbkF	0.20	0.14	79.1	2.03	1.01	1.33E+00
benzo[j]fluoranthene*	BjF	0.01	0.01	79.1	0.60	1.26	1.33E+00
benz[a&e]pyrene	BaeP	0.13	0.08	94.6	2.05	1.26	6.52E+00
perylene*	Per	0.01	0.00	94.6	1.06	1.48	6.52E+00
indeno[1,2,3-cd]pyrene	IP	0.05	0.04	99.3	2.24	0.84	5.22E+01
benzo[ghi]perylene	BP	0.12	0.09	99.8	2.30	0.84	2.57E+02
dibenz[ah]anthracene*	DahA	0.01	0.01	99.3	1.35	1.28	5.29E+01
picene*	Pic	0.01	0.01	99.3	1.13	1.26	5.29E+01
coronene	Cor	0.07	0.05	100	1.59	0.95	1.01E+04
methyl-202-PAH sum	M-202	8.83	6.78	4.02	1.70	0.82	1.19E-02
retene*	Ret	1.80	0.91	10.6	1.54	1.52	3.43E-02
methyl-228-PAH sum	M-228	0.15	0.11	58.8	2.14	0.95	4.72E-01

* Species not included for PMF analysis.

Table S3. Continued

	Abbreviation	Mean	Median	Mean fraction (%)	CV	S/N	$K_{p,om}$ (m ³ µg ⁻¹)
<i>Oxy-PAHs</i>							
acenaphthenone*	Ace-O	411	194	0.04	0.63	1.13	1.14E-04
fluorenone*	Flu-O	433	312	0.12	0.83	0.97	3.24E-04
1H-phenalen-1-one*	Phe-O	283	161	0.15	1.66	1.21	4.09E-04
xanthone*	Xan	43.6	34.1	0.58	2.02	0.82	1.64E-03
1,8-naphthalic anhydride	Nap-DO	54.2	46.9	0.67	2.02	0.57	1.88E-03
anthracene-9,10-dione	Ant-DO	18.2	13.8	2.73	2.01	0.85	7.90E-03
benz[de]anthracene-7-one	BaA-O	0.20	0.16	25.5	2.32	0.78	1.02E-01
<i>Steranes</i>							
20R-abb & 20S-aaa-cholestane	27-RS-C	0.14	0.11	90.4	2.40	0.72	3.50E+00
20R & S-abb-methylcholestane	28-RS-M	0.09	0.07	96.3	2.52	0.96	9.98E+00
20R & S-abb-ethylcholestane	29-RS-E	0.11	0.08	98.6	2.44	0.99	2.84E+01
a-22,29,30-trisnorhopane	TS	0.08	0.07	90.4	2.50	0.79	3.46E+00
ba-30-norhopane	ba-N	0.27	0.21	98.6	2.33	0.98	2.80E+01
ab-hopane	ab-H	0.19	0.14	99.5	2.20	1.17	7.99E+01
22S-ab-30-homohopane	31abS	0.08	0.06	99.8	2.26	1.23	2.28E+02
22R-ab-30-homohopane	31abR	0.06	0.04	99.8	2.17	1.13	2.28E+02
22S-ab-30-bishomohopane	32abS	0.05	0.04	99.9	2.16	1.08	6.50E+02
22R-ab-30-bishomohopane	32abR	0.04	0.03	99.9	2.10	1.09	6.50E+02
<i>Alkanoic acids</i>							
dodecanoic acid	C12:0	536	405	0.92	1.73	0.83	2.62E-03
tridecanoic acid*	C13:0	24.8	13.3	2.57	0.93	1.14	7.46E-03
tetradecanoic acid*	C14:0	96.4	66.4	6.89	1.68	1.14	2.12E-02
pentadecanoic acid*	C15:0	8.74	6.16	17.0	1.36	1.06	6.03E-02
hexadecanoic acid	C16:0	66.8	40.5	35.6	1.65	1.25	1.72E-01
heptadecanoic acid*	C17:0	1.34	0.94	59.3	0.73	1.09	4.89E-01
octadecanoic acid	C18:0	16.4	9.48	79.5	1.47	1.49	1.39E+00
oleic acid*	C18:1	1.14	0.16	82.9	1.42	2.88	1.75E+00
<i>Sterols and methoxyphenols</i>							
cholesterol*	Cho	0.30	0.13	100	0.96	1.27	8.77E+02
stigmasterol*	Sti	0.32	0.17	100	1.13	1.44	8.99E+03
vanillin*	Van	275	151	0.62	1.33	1.60	1.74E-03
acetovanillone*	Acv	70.8	30.3	0.62	0.96	1.56	1.75E-03
coniferaldehyde*	Con	10.5	3.68	5.86	1.47	2.29	1.77E-02
syringaldehyde*	Syr	4.43	0.99	16.2	1.37	2.65	5.63E-02
acetosyringone*	Ace	1.07	0.23	16.4	0.72	2.12	5.67E-02

Table S4.

Statistics for the total concentration of each SVOC estimated for sampling days with ambient temperature above 20 °C (Hot period).

	Abbreviation	Mean	Median	Mean fraction (%)	CV	S/N	$K_{p,om}$ ($m^3 \mu g^{-1}$)
Bulk species ($\mu g m^{-3}$)							
Mass*		7.79	7.53		0.38	4.28	
Nitrate*	Nitr	0.16	0.14		0.76	1.27	
Sulfate	Sulf	1.22	1.11		0.46	14.0	
Ammonium*	Ammo	0.51	0.48		0.54	10.3	
EC		0.46	0.44		0.42	5.81	
OC1*		1.48	1.46		0.25	4.45	
OC2		0.86	0.84		0.38	3.85	
OC3		0.52	0.50		0.30	2.13	
OC4*		0.02	0.01		0.86	1.00	
PC		0.45	0.33		0.79	2.24	
Organic molecular makers ($ng m^{-3}$)							
<i>Alkanes</i>							
docosane	C22	76.8	58.4	2.21	2.48	0.85	4.49E-03
tricosane	C23	62.5	47.8	5.67	2.39	0.81	1.21E-02
tetracosane*	C24	13.7	9.13	13.7	2.01	0.94	3.24E-02
pentacosane	C25	8.50	5.80	29.2	2.22	0.84	8.69E-02
hexacosane	C26	1.41	1.11	51.2	1.97	0.74	2.33E-01
heptacosane	C27	1.44	1.26	72.8	2.55	0.54	6.26E-01
octacosane	C28	0.52	0.40	87.3	1.85	0.85	1.68E+00
nonacosane	C29	2.38	1.99	94.7	2.30	0.70	4.52E+00
triacontane*	C30	0.36	0.24	97.9	1.48	1.14	1.21E+01
hentriacontane*	C31	2.53	1.60	99.2	0.78	1.27	3.26E+01
dotriacontane*	C32	0.67	0.21	99.7	0.54	1.76	8.77E+01
tritriacontane	C33	0.59	0.49	99.9	1.93	0.78	2.36E+02
tetracontane	C34	0.37	0.24	100	1.98	1.06	6.34E+02
pentatriacontane	C35	0.26	0.23	100	1.91	0.78	1.70E+03
hexatriacontane*	C36	0.11	0.09	100	1.43	1.08	4.59E+03
heptatriacontane*	C37	0.07	0.05	100	1.10	1.38	1.23E+04
octatriacontane*	C38	0.06	0.03	100	0.87	1.41	3.32E+04
nonatriacontane*	C39	0.06	0.04	100	0.89	1.06	8.94E+04
tetracontane*	C40	0.04	0.03	100	0.76	1.16	2.41E+05
pentadecylcyclohexane	cycC21	16.9	9.94	0.88	2.03	1.22	1.75E-03
nonadecylcyclohexane*	cycC25	0.41	0.36	30.1	1.80	0.62	9.06E-02
<i>PAHs</i>							
fluoranthene	Flu	20.4	15.6	0.65	1.76	0.82	1.29E-03
pyrene	Pyr	2.49	1.92	2.85	1.76	0.87	5.80E-03
benzo[ghi]fluoranthene	BghiF	0.17	0.13	17.7	1.89	0.81	4.35E-02
cyclopenta[cd]pyrene*	C-pyr	0.04	0.02	21.5	1.51	2.04	5.57E-02
benz[a]anthracene	BaA	0.12	0.07	17.0	1.70	1.45	4.17E-02
chrysene/triphenylene*	CT	0.65	0.49	17.0	2.61	1.22	4.17E-02
benzo[b&k]fluoranthene	BbkF	0.16	0.11	59.0	1.78	1.97	3.13E-01
benzo[j]fluoranthene*	BjF	0.01	0.01	59.0	0.55	1.20	3.13E-01
benz[a&e]pyrene	BaeP	0.07	0.05	85.9	1.68	1.80	1.40E+00
perylene*	Per	0.01	0.01	85.9	0.78	2.86	1.40E+00
indeno[1,2,3-cd]pyrene	IP	0.03	0.02	97.8	1.95	2.11	1.05E+01
benzo[ghi]perylene	BP	0.07	0.05	99.5	2.09	1.44	4.74E+01
dibenz[ah]anthracene*	DahA	0.01	0.00	97.7	0.88	3.33	1.01E+01
picene*	Pic	0.01	0.00	97.7	0.92	8.60	1.01E+01
coronene	Cor	0.04	0.03	100	1.57	1.95	1.60E+03
methyl-202-PAH sum	M-202	12.2	9.23	1.73	1.64	0.90	3.47E-03
retene*	Ret	1.59	0.81	4.28	1.21	1.52	8.91E-03
methyl-228-PAH sum*	M-228	0.16	0.13	34.8	2.00	0.97	1.12E-01

* Species not included for PMF analysis.

Table S4. Continued

	Abbreviation	Mean	Median	Mean fraction (%)	CV	S/N	$K_{p, om}$ ($m^3 \mu g^{-1}$)
<i>Oxy-PAHs</i>							
acenaphthene*	Ace-O	442	91.0	0.02	0.55	1.62	4.65E-05
fluorene*	Flu-O	518	220	0.06	0.73	1.60	1.24E-04
1H-phenalen-1-one*	Phe-O	451	198	0.08	1.68	1.58	1.59E-04
xanthone*	Xan	91.5	78.5	0.30	2.05	0.69	5.83E-04
1,8-naphthalic anhydride*	Nap-DO	138	114	0.36	1.99	0.63	7.13E-04
anthracene-9,10-dione	Ant-DO	45.4	36.9	1.45	2.00	0.74	2.88E-03
benz[de]anthracene-7-one*	BaA-O	0.22	0.18	13.0	2.18	0.74	3.00E-02
<i>Steranes</i>							
20R-abb & 20S-aaa-cholestane	27-RS-C	0.19	0.18	76.5	2.23	0.44	7.40E-01
20R & S-abb-methylcholestane	28-RS-M	0.08	0.08	89.4	2.56	0.43	1.99E+00
20R & S-abb-ethylcholestane	29-RS-E	0.09	0.08	95.7	2.14	0.44	5.33E+00
a-22,29,30-trisnorhopane	TS	0.11	0.10	77.4	2.37	0.43	7.72E-01
ba-30-norhopane	ba-N	0.25	0.23	95.9	2.22	0.42	5.56E+00
ab-hopane	ab-H	0.15	0.14	98.4	2.07	0.44	1.49E+01
22S-ab-30-homohopane	31abS	0.06	0.06	99.4	2.09	0.46	4.01E+01
22R-ab-30-homohopane	31abR	0.05	0.04	99.4	1.96	0.50	4.01E+01
22S-ab-30-bishomohopane	32abS	0.04	0.04	99.8	1.99	0.49	1.08E+02
22R-ab-30-bishomohopane	32abR	0.04	0.03	99.8	1.92	0.53	1.08E+02
<i>Alkanoic acids</i>							
dodecanoic acid*	C12:0	1662	1180	0.40	1.67	1.02	7.96E-04
tridecanoic acid*	C13:0	71.5	36.6	1.07	0.84	1.25	2.13E-03
tetradecanoic acid*	C14:0	407	301	2.80	1.94	0.84	5.72E-03
pentadecanoic acid*	C15:0	34.7	23.7	7.12	1.45	0.93	1.53E-02
hexadecanoic acid*	C16:0	188	120	16.8	1.51	0.98	4.11E-02
heptadecanoic acid*	C17:0	4.38	3.00	34.4	0.64	0.95	1.10E-01
octadecanoic acid*	C18:0	21.6	14.9	57.4	1.47	0.88	2.96E-01
oleic acid*	C18:1	0.64	0.24	63.1	0.86	2.91	3.79E-01
<i>Sterols and methoxyphenols</i>							
cholesterol*	Cho	0.24	0.13	99.8	0.78	1.29	1.50E+02
stigmasterol*	Sti	0.33	0.13	100	0.69	1.70	1.38E+03
vanillin*	Van	194	123	0.32	0.93	1.71	6.26E-04
acetovanillone*	Acv	52.7	8.50	0.35	0.53	1.94	6.82E-04
coniferaldehyde*	Con	7.81	3.24	2.83	0.94	1.45	5.75E-03
syringaldehyde*	Syr	3.76	0.68	8.08	0.99	3.53	1.75E-02
acetosyringone*	Ace	2.66	0.28	8.75	0.52	1.85	1.90E-02

Table S5. Mean particle-phase fractions of selected SVOCs and data from other field studies.

	This study (PM _{2.5})				Fraser et al. (1997,1998) (PM _{1.6})	Simcik et al. (1997, 1998) (TSP)			Tsapakis and Stephanou (2005) (TSP)	Mandalakis et al. (2002) (TSP)
	Whole	Cold	Warm	Hot	Los Angeles, Summer	Chicago, Winter	Chicago, Summer	Lake Michigan, Summer	Heraklion (Greece), Annual	Athens (Greece), Summer
Average Temp. (°C)	14	3.3	15	24	27	2.7	23	22	17	28
Sample No.	970	364	318	288	32	1-4	1-18	2-15	16	4
<i>Alkanes</i>										
docosane	16	36	6.4	2.2	2.8					17
tricosane	29	58	16	5.7	10					26
tetracosane	44	78	34	14	25					36
pentacosane	61	90	57	29	32					56
hexacosane	77	96	78	51	44					62
heptacosane	88	99	90	73	72					81
octacosane	98	100	96	87	94					66
nonacosane	98	100	99	95	100					87
triacontane	99	100	100	98	100					65
hentriacontane	100	100	100	99	100					91
dotriacontane	100	100	100	100	100					78
tritriacontane	100	100	100	100	100					70
tetratriacontane	100	100	100	100	100					
pentatriacontane	100	100	100	100	100					
hexatriacontane	100	100	100	100	100					
<i>PAHs</i>										
fluoranthene	4.1	9.2	1.5	0.65	0.71	55	17	9.7	3.7	6.4
pyrene	15	31	6.7	2.8	1.0	54	20	14	4.7	9.0
benzo[ghi]fluoranthene	44	74	35	18	18					
cyclopenta[cd]pyrene	49	77	40	22	35				32	
benz[a]anthracene	45	75	35	17	60	95	81	49	57	41
chrysene/triphenylene	45	75	35	17	44	92	72	40	53	45
benzo[b&k]fluoranthene	79	96	79	59	100	94	93	77	94	96
benzo[j]fluoranthene	79	96	79	59	100					
benz[a&e]pyrene	94	99	95	86	100	95	90	88	92	99
perylene	94	99	95	86	100				91	100
indeno[1,2,3-cd]pyrene	99	100	99	98	100				98	100
benzo[ghi]perylene	100	100	100	100	100	96	95	92	97	100
dibenz[ah]anthracene	99	100	99	98					100	100
coronene	100	100	100	100					100	100
retene	21	43	11	4.3					10	

Table S5. Continued

	This study (PM _{2.5})				Fraser et al. (1997,1998) (PM _{1.6})	Mandalakis et al. (2002) (TSP)
	Whole	Cold	Warm	Hot	Los Angeles, Summer	Athens (Greece), Summer
Average Temp. (°C)	14	3.3	15	24	27	28
Sample No.	970	364	318	288	32	4
<i>Sterane and hopanes</i>						
20R-abb & 20S-aaa-cholestane	89	98	90	76	100	
a-22,29,30-trisnorhopane	89	98	90	77	100	40
ab-hopane	99	100	100	98	100	83
22S-ab-30-homohopane	100	100	100	100	100	93
22R-ab-30-homohopane	100	100	100	100	100	92
22S-ab-30-bishomohopane	100	100	100	100	100	100
22R-ab-30-bishomohopane	100	100	100	100	100	100

Table S6.

Correlation coefficients of factor contributions from full data set solution versus meteorological and trace gas measurements.

Factors	Temperature (°C)	Radiance (KW-hr m ⁻²)	RH (%)	Ozone (ppm)	NO _x (ppm)	CO (ppm)
Whole period						
Nitrate	-0.60	-0.46	0.49	-0.51	0.45	0.39
Sulfate	0.15	0.21	0.31	0.04*	-0.07*	-0.05*
<i>n</i> -Alkane	-0.28	-0.22	0.10*	-0.35	0.45	0.43
Sterane	-0.35	-0.32	0.17	-0.47	0.64	0.58
Light SVOCs	0.73	0.50	-0.48	0.34	-0.30	-0.20
PAH	-0.39	-0.34	0.05*	-0.59	0.65	0.62
Bulk carbon	0.39	0.33	-0.22	0.46	-0.10*	0.05*
Cold period						
Nitrate	-0.38	-0.10*	0.40	-0.40	0.31	0.29
Sulfate	-0.22	0.08*	0.40	-0.07*	-0.03*	-0.04*
<i>n</i> -Alkane	-0.19	-0.16	-0.11*	-0.33	0.47	0.43
Sterane	-0.09*	-0.28	-0.01*	-0.50	0.57	0.54
Light SVOCs	0.61	0.15	-0.34	0.24	-0.21	-0.15
PAH	0.03*	-0.06*	-0.30	-0.46	0.57	0.60
Bulk carbon	0.15	0.14	-0.16	-0.15	0.28	0.33
Warm period						
Nitrate	-0.20	-0.18	0.38	-0.23	0.23	0.27
Sulfate	0.16	0.16	0.43	0.12*	-0.16	-0.04*
<i>n</i> -Alkane	-0.05*	-0.06*	-0.03*	-0.05*	0.22	0.17
Sterane	-0.14*	-0.10*	-0.01*	-0.21	0.60	0.55
Light SVOCs	0.35	0.23	-0.33	0.05*	-0.08*	-0.06*
PAH	-0.25	-0.15*	-0.10*	-0.43	0.62	0.61
Bulk carbon	0.19	0.09*	0.28	0.08*	0.18	0.25
Hot period						
Nitrate	-0.02*	-0.04*	0.03*	0.03*	0.08*	0.06*
Sulfate	0.07*	0.11*	0.26	0.18	-0.09*	-0.03*
<i>n</i> -Alkane	-0.01*	0.08*	-0.03*	0.05*	0.31	0.16
Sterane	0.01*	0.03*	0.01*	-0.00*	0.36	0.34
Light SVOCs	0.16	-0.06*	-0.45	-0.48	0.01*	0.03*
PAH	-0.15*	-0.15*	-0.11*	-0.46	0.44	0.31
Bulk carbon	0.21	0.17	0.10*	0.36	0.21	0.39

* Correlation is not significant at the 0.01 level (2-tailed), and the absolute *r* values equal or higher than 0.40 are in bold.

Table S7.

Correlation coefficients of factor contributions from sub-data set solutions versus meteorological and trace gas measurements.

Factors	Temperature (°C)	Radiance (KW-hr m ⁻²)	RH (%)	Ozone (ppm)	NO _x (ppm)	CO (ppm)
Cold period						
Nitrate	-0.43	-0.09*	0.39	-0.40	0.32	0.29
Sulfate	-0.27	0.07*	0.42	-0.09*	-0.02*	-0.03*
<i>n</i> -Alkane	-0.22	-0.11*	-0.09*	-0.32	0.43	0.39
Sterane	-0.11*	-0.28	-0.00*	-0.48	0.53	0.50
Light SVOCs	0.61	0.17	-0.40	0.26	-0.22	-0.15
PAH	-0.10*	-0.13*	-0.24	-0.44	0.49	0.52
Bulk carbon	-0.04*	0.03*	-0.14*	-0.51	0.76	0.76
Warm period						
Nitrate	-0.06*	-0.03*	0.37	-0.23	0.24	0.29
Sulfate	0.19	0.21	0.40	0.16	-0.22	-0.10*
<i>n</i> -Alkane	-0.04*	-0.06*	-0.01*	-0.04*	0.22	0.16
Sterane	-0.12*	-0.03*	-0.01*	-0.20	0.58	0.53
Light SVOCs	0.33	0.19	-0.39	0.11*	-0.17	-0.15
PAH	-0.27	-0.21	-0.12*	-0.43	0.61	0.61
Bulk carbon	0.23	0.10*	0.26	0.03*	0.22	0.28
Hot period						
Sulfate	0.08*	0.13*	0.29	0.23	-0.11*	-0.07*
<i>n</i> -Alkane	0.02*	0.11*	-0.01*	0.16	0.15*	0.16
Sterane	-0.02*	0.05*	0.16	0.13*	0.20	0.24
Light SVOCs	0.07*	0.02*	-0.36	-0.46	0.01*	-0.06*
PAH	-0.19	-0.08*	-0.13*	-0.44	0.47	0.32
Bulk carbon	0.14*	0.05*	0.07*	0.16	0.31	0.47
Medium <i>n</i> -alkane	0.59	0.26	-0.45	0.15*	-0.20	-0.04*

* Correlation is not significant at the 0.01 level (2-tailed), and the absolute *r* values equal or higher than 0.40 are in bold.

Figure Captions

- Fig. S1 – Median PMF factor profiles for the full data set solution (shaded bars). The whiskers represent the variability in factor profile derived from bootstrapped PMF solutions (+ 1 SD). The bars are shaded to show compound class separations.
- Fig. S2 – Median PMF factor contributions for the full data set solution (black points). The gray bars represent the variability in the estimation of factor contribution from bootstrapped PMF solutions (+/- 1 SD).
- Fig. S3 – Day of the week box plots for the factor contributions of full data set solution. The boxes depict the median (dark line), inner quartile range (shaded box), 10th and 90th percentiles (whiskers) and the mean (asterisk). The dashed line across the plot is the overall median. The individual median values and the number of points contained within each box are listed below the box.
- Fig. S4 – Median PMF factor profiles for the cold period sub-data set solution (shaded bars). The whiskers represent the variability in factor profile derived from bootstrapped PMF solutions (+ 1 SD). The bars are shaded to show compound class separations.
- Fig. S5 – Median PMF factor profiles for the warm period sub-data set solution (shaded bars). The whiskers represent the variability in factor profile derived from bootstrapped PMF solutions (+ 1 SD). The bars are shaded to show compound class separations.
- Fig. S6 – Median PMF factor profiles for the hot period sub-data set solution (shaded bars). The whiskers represent the variability in factor profile derived from bootstrapped PMF solutions (+ 1 SD). The bars are shaded to show compound class separations.

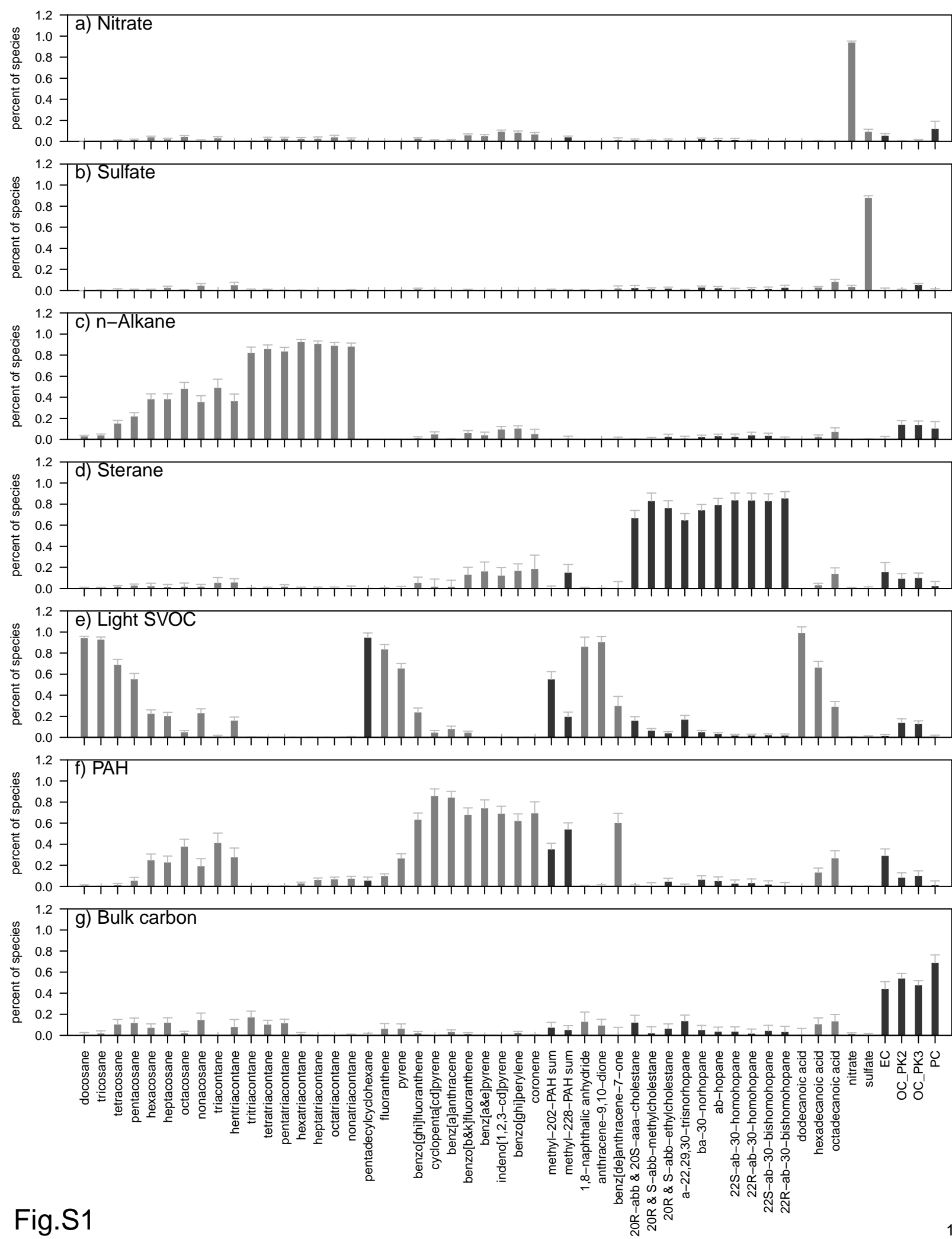


Fig.S1

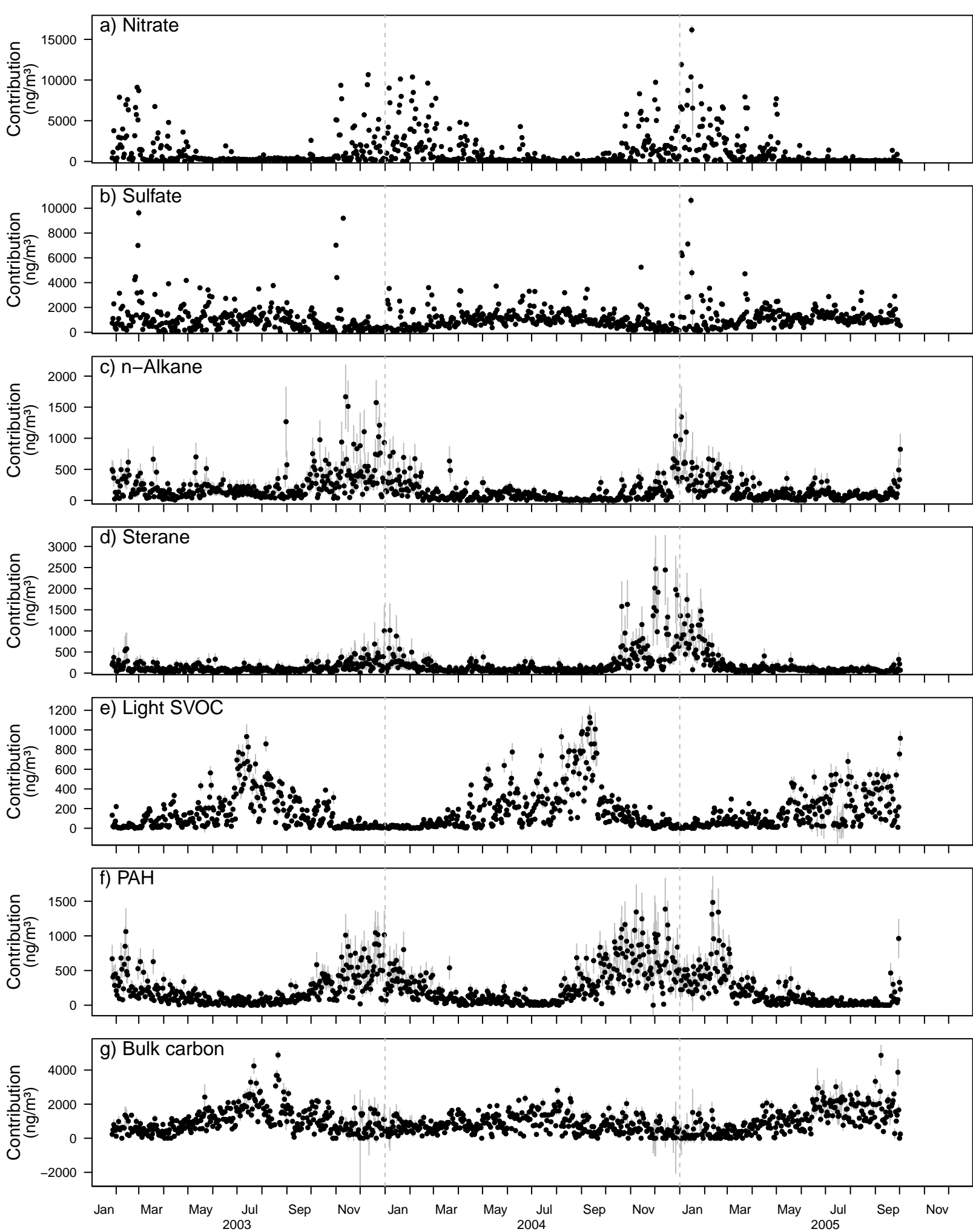


Fig.S2

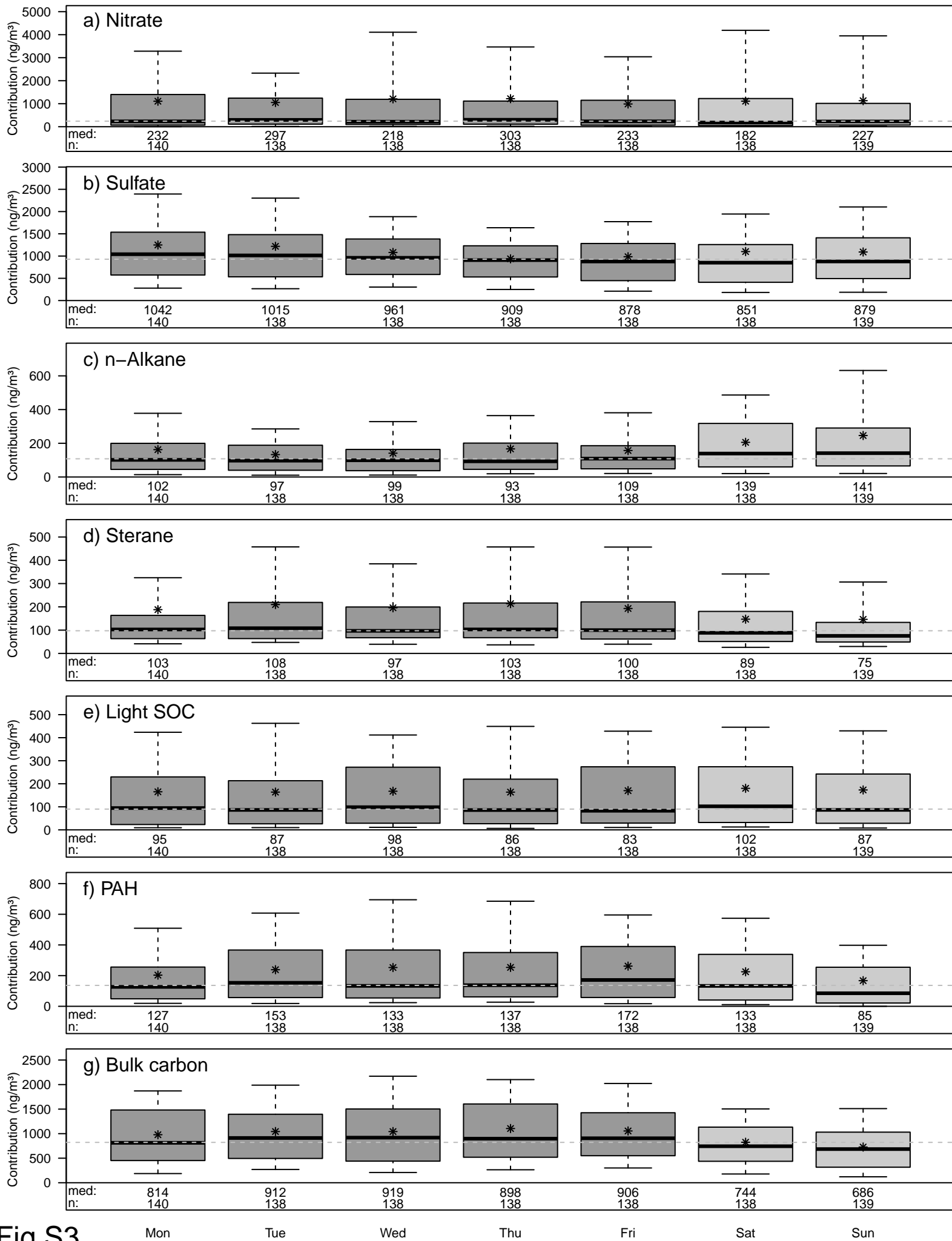


Fig.S3

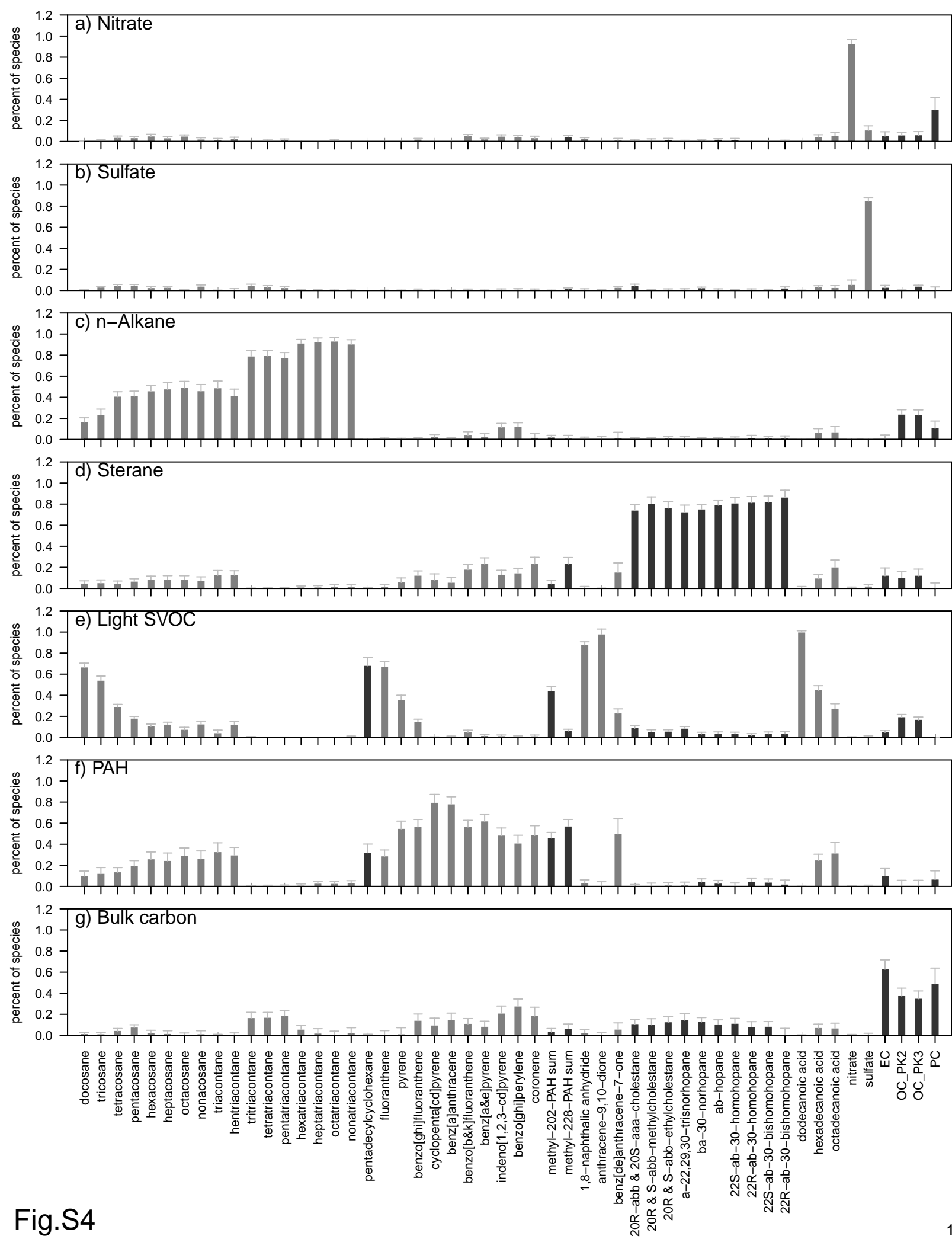


Fig.S4

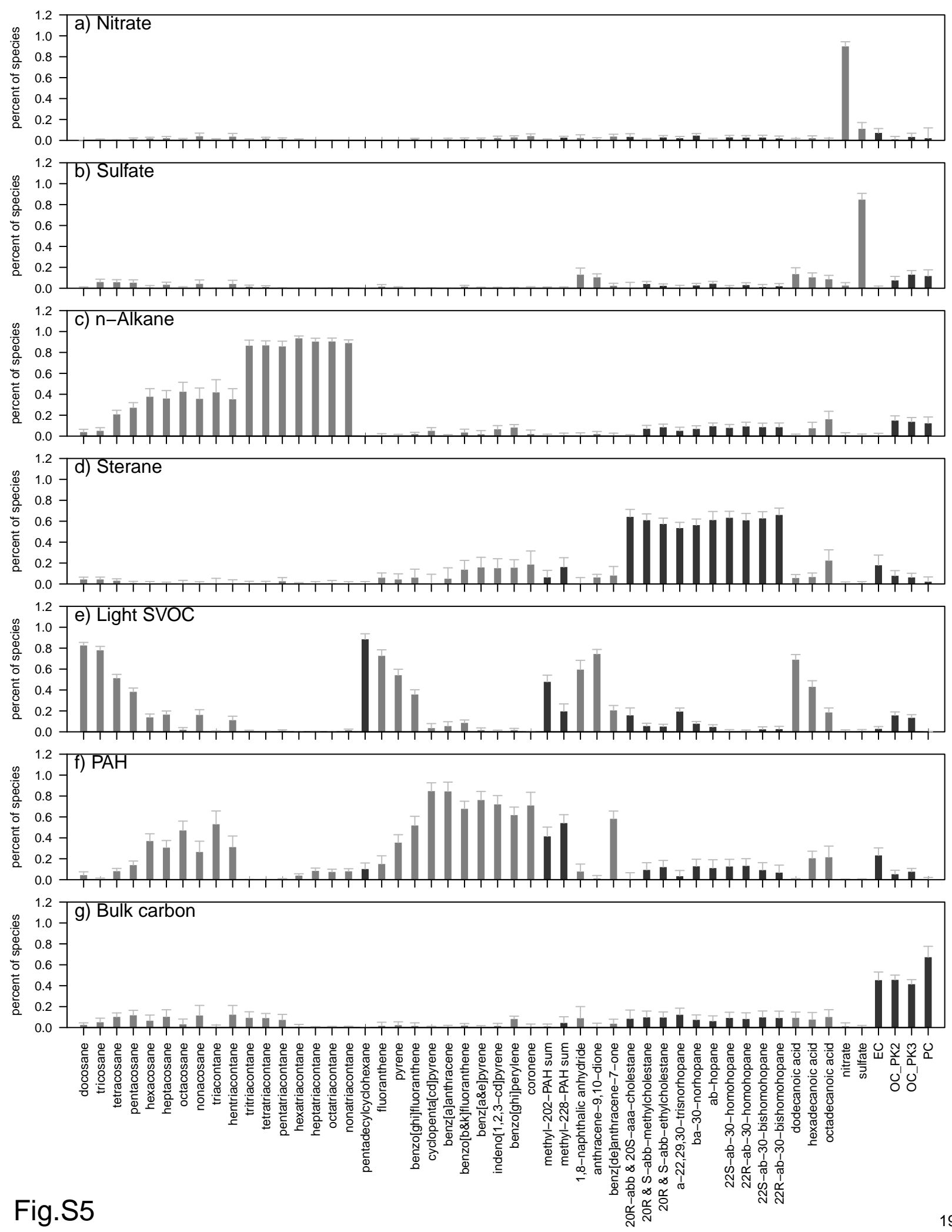


Fig.S5

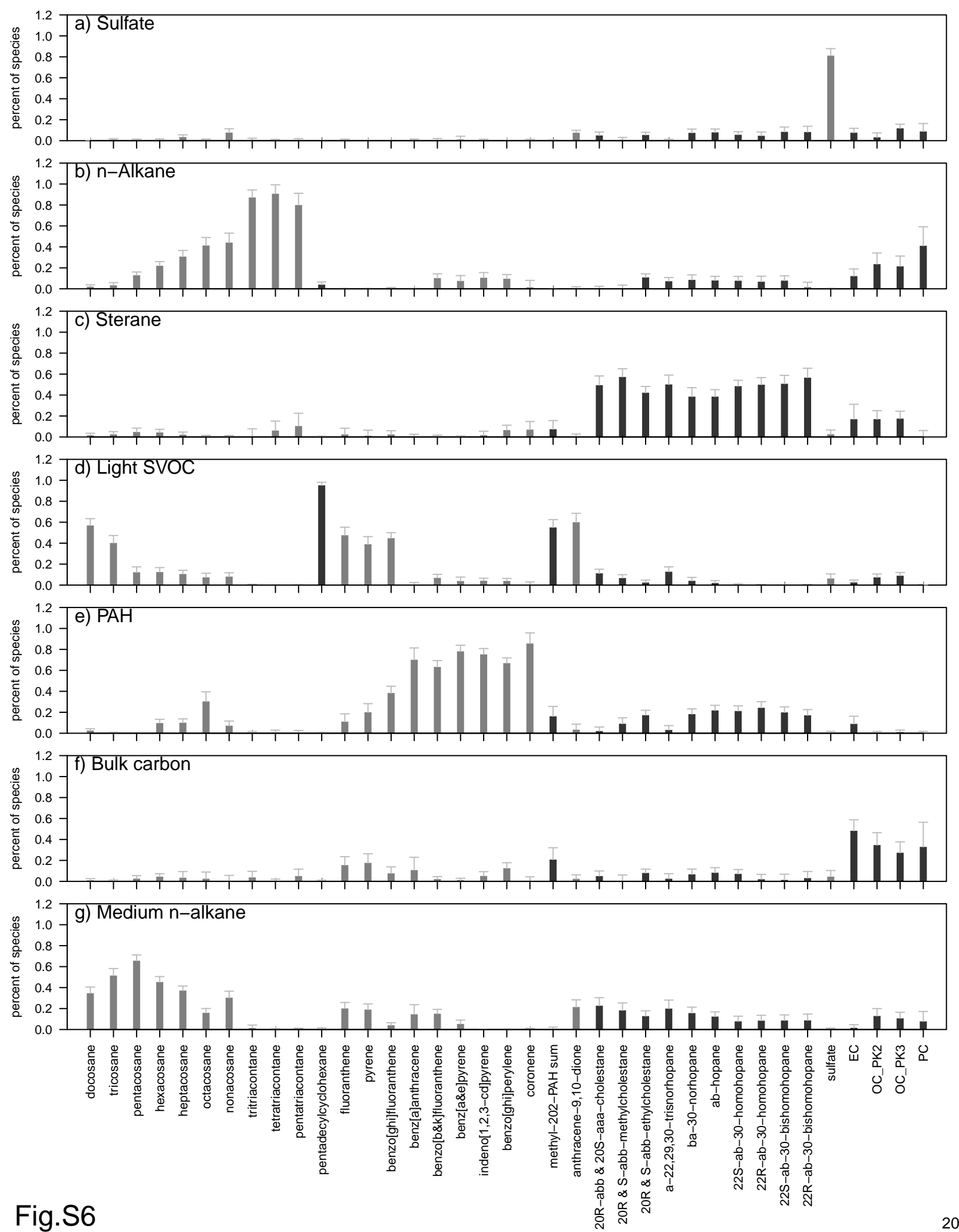


Fig.S6

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