



POSITIVE MATRIX FACTORIZATION (PMF) 5.0



AGENDA

- **Source apportionment analysis**
- **Positive matrix factorization (PMF) model**
- **Common tracers in the atmosphere**
- **Examples**
- **Final tips & takeaways**

What is source apportionment in atmospheric sciences?

With source apportionment analysis we will know:

- Where does this pollution come from?
- How much of it comes from traffic, industry, agriculture, natural sources, etc.?

Source apportionment is critically important in atmospheric sciences because it helps identify and quantify the contributions of different emission (pollution) sources to air quality.



Why is important the source apportionment in atmospheric sciences?

1. Effective Air Quality Management

Understanding the sources of pollutants (e.g., vehicles, industry, agriculture, wildfires) allows policymakers to target the most significant contributors with regulations or interventions.



2. Public Health Protection

Different pollution sources can have varying health impacts. For example, fine particles from diesel exhaust may be more harmful than those from natural dust. Apportionment helps prioritize actions to reduce the most toxic sources.

3. Model Validation and Improvement

Chemical transport and air quality models rely on ***assumptions about emissions***. Source apportionment studies provide ***real-world data*** to validate and refine these models.

Why is important the source apportionment in atmospheric sciences?

4. Climate Change Implications

Some pollutants affect both air quality and climate (e.g., black carbon, ozone). Source apportionment informs strategies that co-benefit climate and air quality goals.



5. Global Pollution

Air pollution doesn't have borders. Apportionment can distinguish between local and long-range transported pollution, guiding diplomatic or regional cooperation.

WHAT IS THE POSITIVE MATRIX FACTORIZATION (PMF) MODEL?

WHAT IS THE POSITIVE MATRIX FACTORIZATION (PMF) MODEL?

The PMF Model can analyze a wide range of environmental sample data: sediments, wet deposition, surface water, and ambient air.

EPA's PMF Model reduces the large number of variables in complex analytical data sets to combinations of species called source types and source contributions.

The source types are identified by comparing them to measured profiles. Source contributions are used to determine how much each source contributed to a sample. In addition, PMF provides robust uncertainty estimates and diagnostics.

<https://www.epa.gov/air-research/positive-matrix-factorization-model-environmental-data-analyses>



What is the Positive Matrix Factorization (PMF) Model?

- PMF is a **receptor model** that analyzes measured concentrations of pollutants (e.g., PM_{2.5} chemical components) at a given location.
- It statistically decomposes this data into a set of **source profiles** and **contributions** over time—without requiring prior knowledge of the sources.

How it works:

- The observed concentration matrix **X** is approximated by multiplying two matrices:

$$\mathbf{X} = \mathbf{G} \cdot \mathbf{F} + \mathbf{E}$$

- **G** = Contributions of each source to each sample (time series)
- **F** = Chemical profiles of sources (what each source emits)
- **E** = Residual (unexplained part)

Cons:

- **Requires expertise to interpret results**
- Sometimes sensitive to missing or noisy data

HOW DOES THE MODEL WORK?

Input:

PMF users provide files of sample species **concentrations** and **uncertainties** and the number of sources. The model calculates source profiles or fingerprints, source contributions, and source profile uncertainties. PMF Model results are constrained to provide positive source contributions, and the uncertainty weighted difference between the observed and predicted species concentration is minimized.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1		Aluminum	Ammonium	Bromine	Calcium	Chlorine	Copper	EC	Iron	Lead	Manganese	Nickel	Nitrate	OC
2	DATE	µg/m ³												
3	2/9/2000	0.0201	3.6020	0.0107	0.0676	0.0647	0.0059	3.1230	0.1497	0.0157	0.0043	0.0577	5.3700	7.3930
4	2/15/2000	0.0057	1.3740	0.0006	0.0325	0.0016	0.0019	1.0710	0.0673	0.0055	0.0004	0.0285	0.8785	3.3310
5	2/27/2000	0.0029	2.1860	0.0028	0.0422	0.0288	0.0028	0.6732	0.0727	0.0073	0.0002	0.0215	3.8820	5.2030
6	3/4/2000	0.0011	0.4501	0.0014	0.0329	0.0024	0.0010	0.5503	0.0483	0.0061	0.0004	0.0188	0.4562	3.6160
7	3/10/2000	0.0075	0.3099	0.0006	0.0247	0.0039	0.0003	0.2869	0.0565	0.0032	0.0016	0.0083	0.6763	2.8140
8	3/22/2000	0.0006	1.1570	0.0033	0.0265	0.0015	0.0029	0.9487	0.0821	0.0044	0.0012	0.0107	1.0670	2.4150
9	4/6/2000	0.0256	1.3520	0.0025	0.0863	0.0026	0.0041	2.1990	0.1492	0.0089	0.0034	0.0254	1.4660	4.7350
10	4/9/2000	0.0165	0.2800	0.0011	0.0263	0.0016	0.0003	0.8535	0.0396	0.0017	0.0019	0.0257	0.2515	1.6760
11	4/12/2000	0.0108	1.1290	0.0026	0.0304	0.0080	0.0046	0.9983	0.0959	0.0042	0.0001	0.0344	1.1900	2.6360
12	4/15/2000	0.0065	1.5640	0.0037	0.1075	0.0296	0.0059	3.1430	0.1976	0.0110	0.0026	0.0437	4.3040	6.9460
13	4/18/2000	0.0072	0.1983	0.0028	0.0351	0.0073	0.0017	0.6603	0.0539	0.0004	0.0027	0.0082	0.6816	1.9990
14	4/21/2000	0.0092	0.1432	0.0022	0.0250	0.0042	0.0023	0.7096	0.0765	0.0003	0.0009	0.0126	0.6017	1.7230
15	4/24/2000	0.0289	0.4066	0.0000	0.0337	0.0007	0.0006	1.1100	0.0830	0.0067	0.0005	0.0256	0.2174	2.4420
16	4/27/2000	0.0033	1.5030	0.0031	0.0329	0.0010	0.0024	1.4970	0.0840	0.0082	0.0013	0.0247	3.3670	3.5360
17	4/30/2000	0.0120	0.5734	0.0021	0.0442	0.0097	0.0022	0.6726	0.0741	0.0025	0.0041	0.0153	0.5117	3.3610
18	5/3/2000	0.0098	1.3200	0.0014	0.0365	0.0039	0.0015	1.1210	0.0735	0.0077	0.0000	0.0056	1.3380	4.2670
19	5/12/2000	0.0209	0.1049	0.0013	0.0394	0.0003	0.0033	1.2070	0.1108	0.0046	0.0000	0.0114	0.6438	3.8460
20	5/15/2000	0.0096	1.1600	0.0010	0.0337	0.0023	0.0002	0.8730	0.0902	0.0064	0.0004	0.0167	0.3547	3.1960
21	5/18/2000	0.0348	2.9630	0.0037	0.1088	0.0083	0.0066	1.9910	0.1519	0.0054	0.0031	0.0166	3.3450	6.1610
22	5/21/2000	0.0008	1.9910	0.0014	0.0409	0.0011	0.0025	0.4828	0.0449	0.0038	0.0018	0.0099	2.0890	2.5760
23	5/24/2000	0.0067	1.8440	0.0010	0.0386	0.0013	0.0005	1.4190	0.0957	0.0045	0.0007	0.0553	1.3390	4.2690

	A	B	C	D	E	F	G	H
1	unc	Aluminum	Ammonium	Arsenic	Barium	Bromine	Calcium	Chlorine
2	2	0.00419	0.0125	0.00098	0.0068	0.0016	0.0038	0.002635
3	10	10	10	10	10	10	10	10
4								

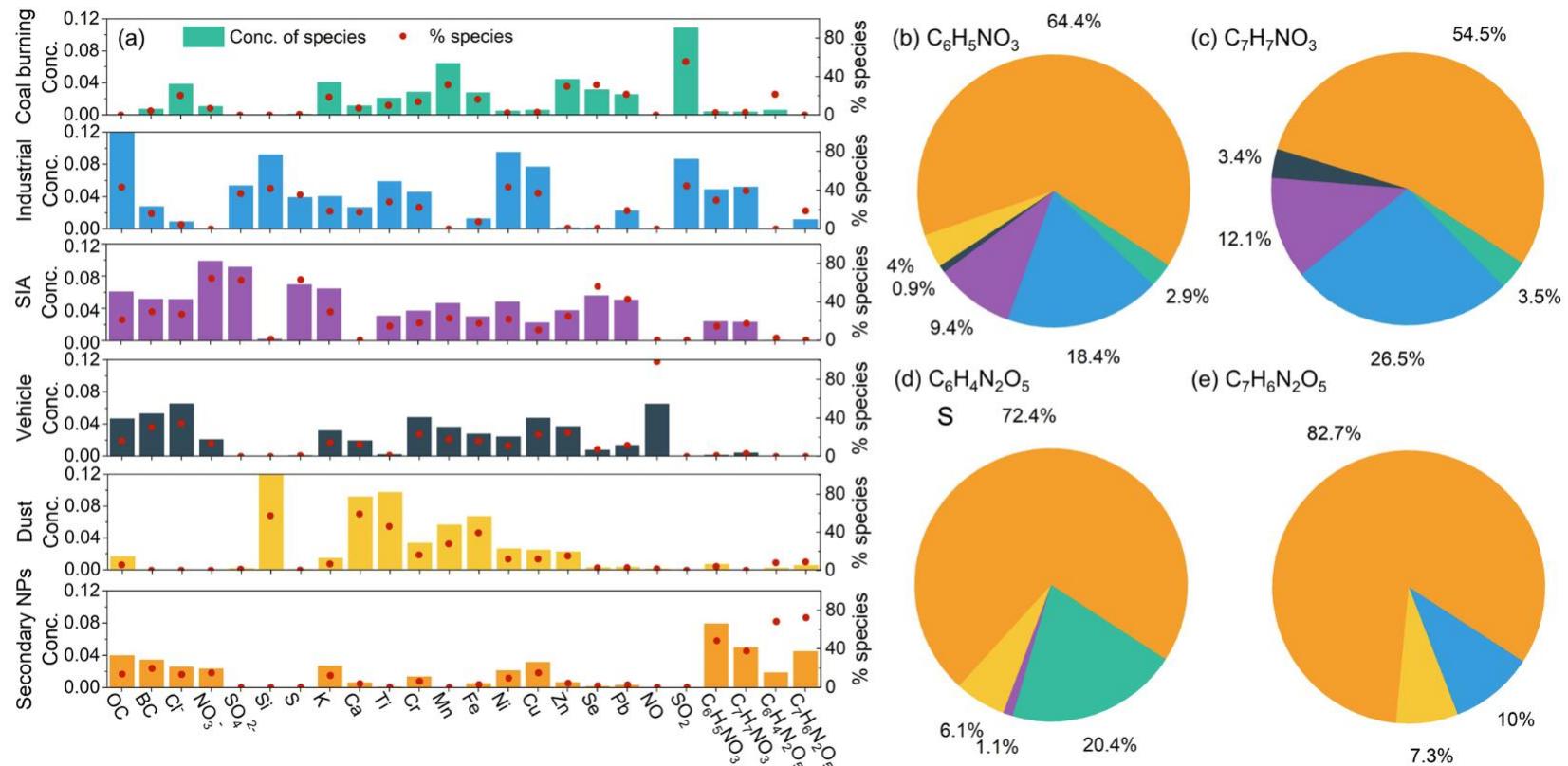
HOW DOES THE MODEL WORK?

Output:

PMF Model software uses graphical user interfaces that ease data input, visualization of model diagnostics, and exporting of results.

The model is free of charge and does not require a license or other software to use.

Algorithms used in the PMF Model have been peer reviewed by leading air and water quality management scientists.



<https://www.epa.gov/air-research/positive-matrix-factorization-model-environmental-data-analyses>

Men Xia et al., 2023, *Journal of Geophysical Research: Atmospheres*
128(22) DOI: 10.1029/2023JD039551

What are the tracers?

In environmental science, tracers or markers are substances or indicators used to track the movement, origin, or fate in natural systems such as water, in atmosphere, or in a biological organism.

Typical characteristic of a tracer:

- The tracer, must be emitted exclusively or predominantly by specific sources, giving those sources a relatively unique chemical signature.
- The tracer compound should be chemically stable in the atmosphere, reacting slowly enough to remain unchanged from the point of emission to the receptor site.
- Ideally, a tracer should not be formed through atmospheric reactions, nor should it volatilize during transport, in order to ensure that mass balance is maintained.

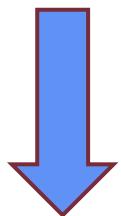


Key tracers in atmospheric sciences

Natural Sources

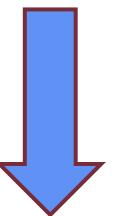


Desert dust



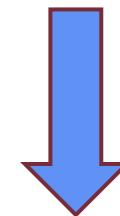
Al, Si, nss-Ca²⁺

Sea salts

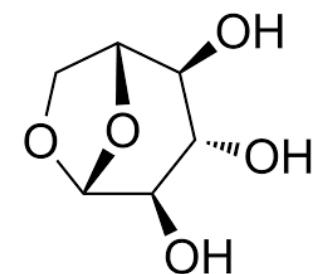


CL, ss-Na⁺

Biomass burning



Levoglucosan, nss-K⁺



$$\text{nss-Ca}^{2+} = \text{Total Ca}^{2+} - \left(\frac{\text{Ca}^{2+}}{\text{Na}^+} \right)_{\text{sea water}} \times \text{Na}_{\text{sample}}^+$$

nss: non-sea salt

$$[\text{nss-Ca}^{2+}] = [\text{Ca}^{2+}] - 0.0383 \times [\text{Na}^+]$$

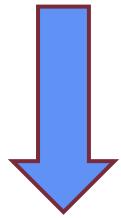
$$[\text{nss-K}^+] = [\text{K}^+] - 0.0371 \times [\text{Na}^+]$$

Key tracers in atmospheric sciences

Natural Sources



Pollen



Sucrose

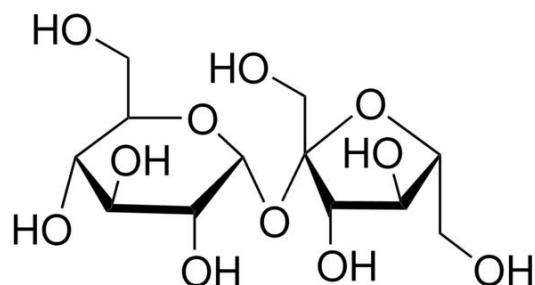
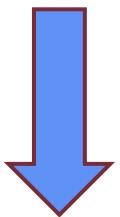
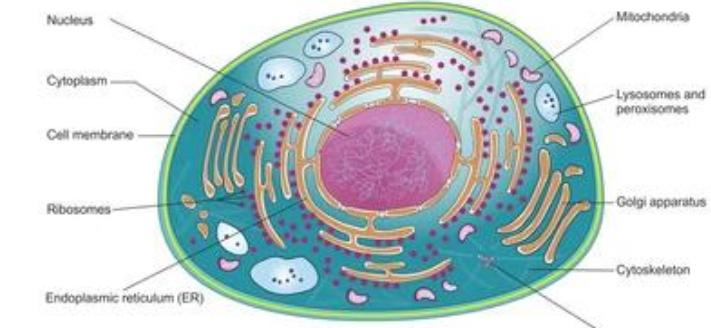
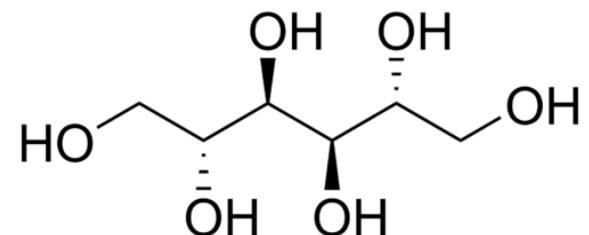


Image Credit: Kateryna Kon/Shutterstock.com

Fungi



Mannitol

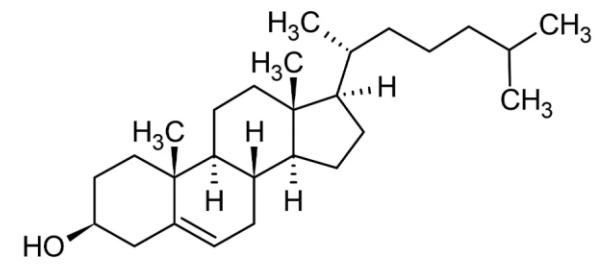


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Mammals cells



Cholesterol

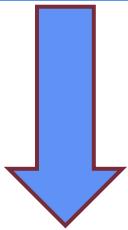


Key tracers in atmospheric sciences

Anthropogenic Sources



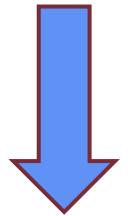
Ship emissions



V and Ni
Emissions from marine
fuel combustion



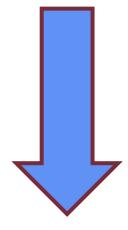
Industry and other
anthropogenic emission



nss- SO_4^{2-} , NO_3^- , Pb, Cd, Cr
Cu, Fe → brake/tires



Industrial Sources



nss- SO_4^{2-} , Pb, Cd, Cr, Zn

$$[\text{nss-}\text{SO}_2^{-4}] = [\text{SO}_2^{-4}]_{\text{total}} - 0.2517 \times [\text{Na}^+]$$

Other Key tracers in atmospheric sciences

Organics markers  Origins	
MSA	Marine SOA
Levoglucosan	Primary biomass burning
1-Nitropyrene (1-NP)	Diesel emission
6H-Dibenzo[b,d]pyran-6-one	SOA PAH
Benzo[a]fluorenone	SOA/POA PAH
Benzo[b]fluorenone	SOA/POA PAH
9-Nitroanthracene	SOA/POA PAH
2-Nitrofluoranthene	SOA PAH
DHOPA	SOA Toluene
4-Methyl-5-nitrocatechol	SOA Phenolic compounds
3-Methyl-5-nitrocatechol	SOA Phenolic compounds
2-Methylerythritol	SOA Isoprene
α -Methylglyceric acid	SOA Isoprene

PMF applications in atmospheric sciences

EXAMPLES

EXAMPLE-1

Identifying the sources of atmospheric organic Phosphorus

npj | climate and atmospheric science

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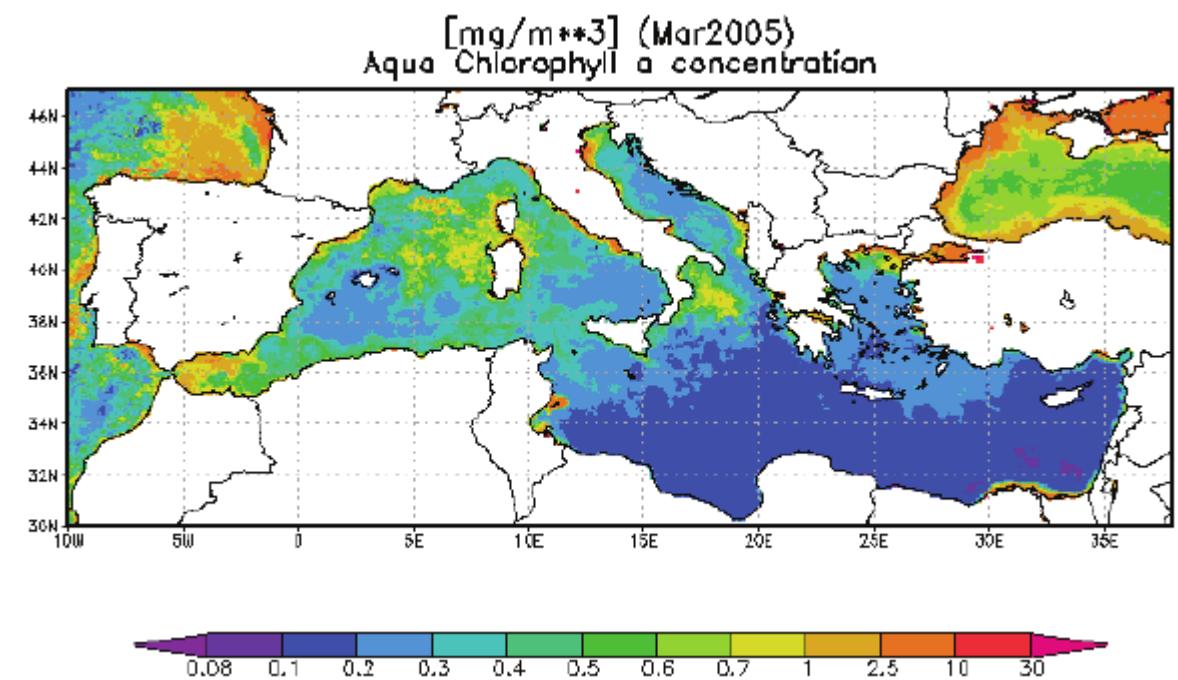
Bioaerosols and dust are the dominant sources of organic P in atmospheric particles

[Kalliopi Violaki](#)✉, [Athanasios Nenes](#), [Maria Tsagkaraki](#), [Marco Paglione](#), [Stéphanie Jacquet](#), [Richard Sempéré](#) & [Christos Panagiotopoulos](#)

• Background of the paper....

Why is important the study of P for Mediterranean sea

- It is known that East MS in P limited, while the atmosphere considered as an important nutrient path for the pelagic marine organisms, especially during stratification period (usually from May-September).
- Decoding the chemical structure of the P fraction could reveal valuable information regarding their bioavailability in the marine environment.
- Understanding better the atmospheric chemistry of P compounds and beyond the biochemical cycle of P.



Scenario B



26%



17%



52%



4.6%



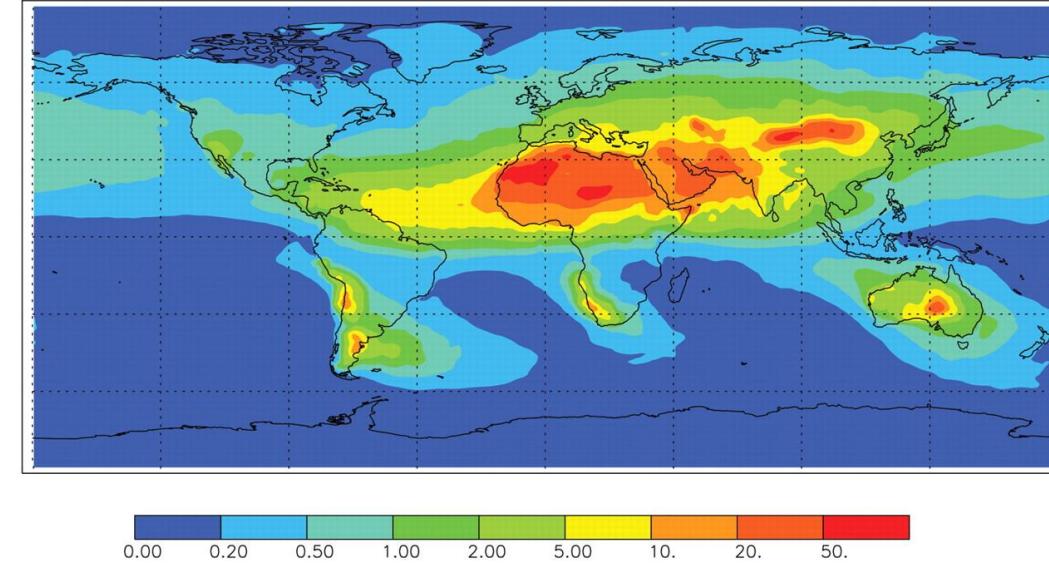
0.2%



Total global P: 3.5 Tg P y⁻¹

The global P sources according to modeling assessment

Average dust deposition (g/m²/year)

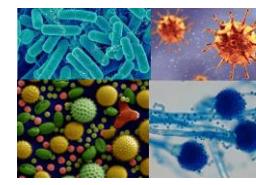


- Mediterranean seems to follow the scenario A due to proximity to Sahara desert.
- Scenario B could be a future scenario or a more regional scenario in areas with high frequency of BB events.
- Is missing the source distribution in org-P and inorg-P, which could explain different processes in P cycle.

Scenario A



84%



12%



2%



2%



0.4%



0.4%



Total global P: 1.37 Tg P y⁻¹

EXAMPLE-1

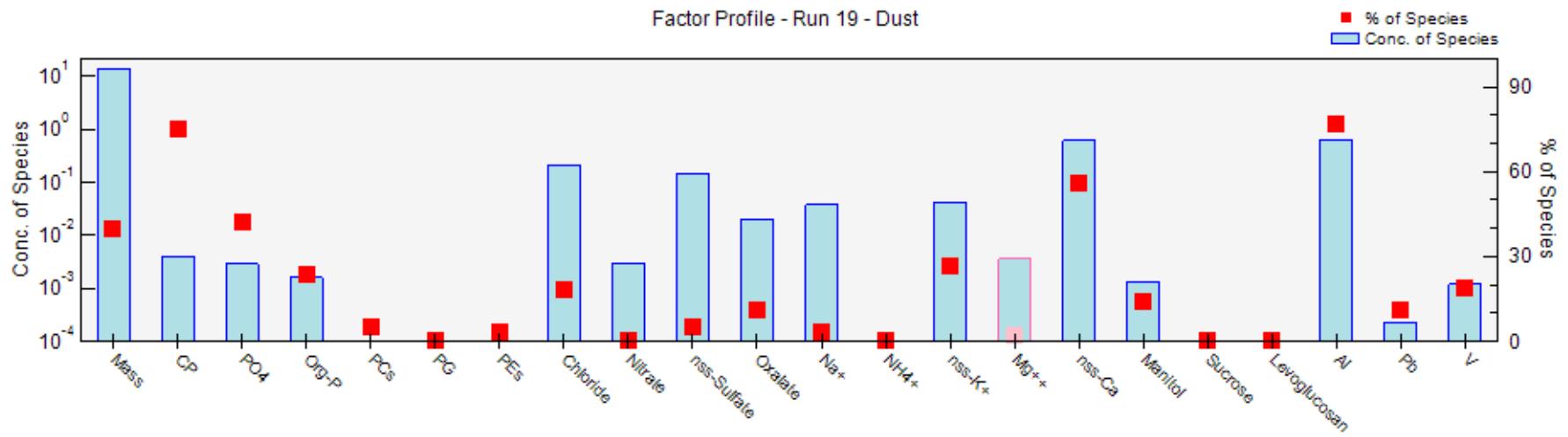
Identifying the sources of atmospheric organic Phosphorus

Supplementary Table 8: Characteristic tracers for the identification of the PMF factors.

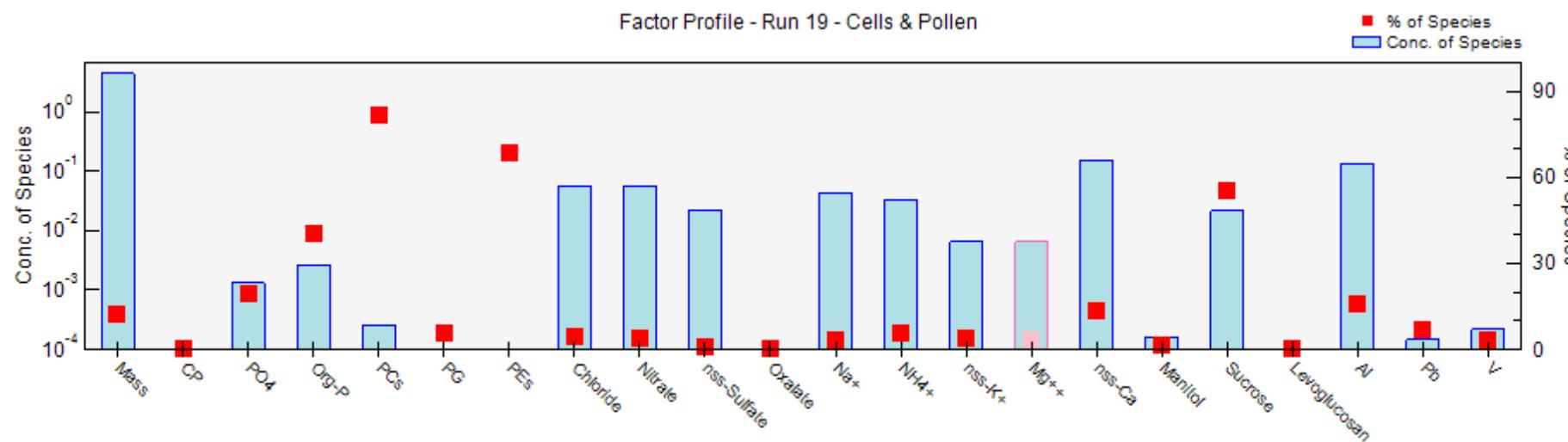
Identified factors	Specific tracers	References
Cells & Pollen	PCs, PEs, sucrose	Womiloju et al. 2003 ² , Fu et al., 2012 ³
Fungi	Mannitol	Fu et al., 2012 ³
Sahara dust	Aluminium, nss-Ca ²⁺	Belis et al., 2019 ⁴
Anthropogenic	Nitrate, Pb, V	Belis et al., 2019 ⁴
Secondary sulfate	Nss-SO ₄ ²⁻ , NH ₄ ⁺	Manousakas et al., 2017 ⁵
Biomass burning	nss-K ⁺ , Levoglucosan	Belis et al., 2019 ⁴
Sea-salts	Cl ⁻ , Mg ²⁺	Belis et al., 2019 ⁴ Manousakas et al., 2017 ⁵

Factors in PMF= Source profile

Sources suggested by PMF 5.0



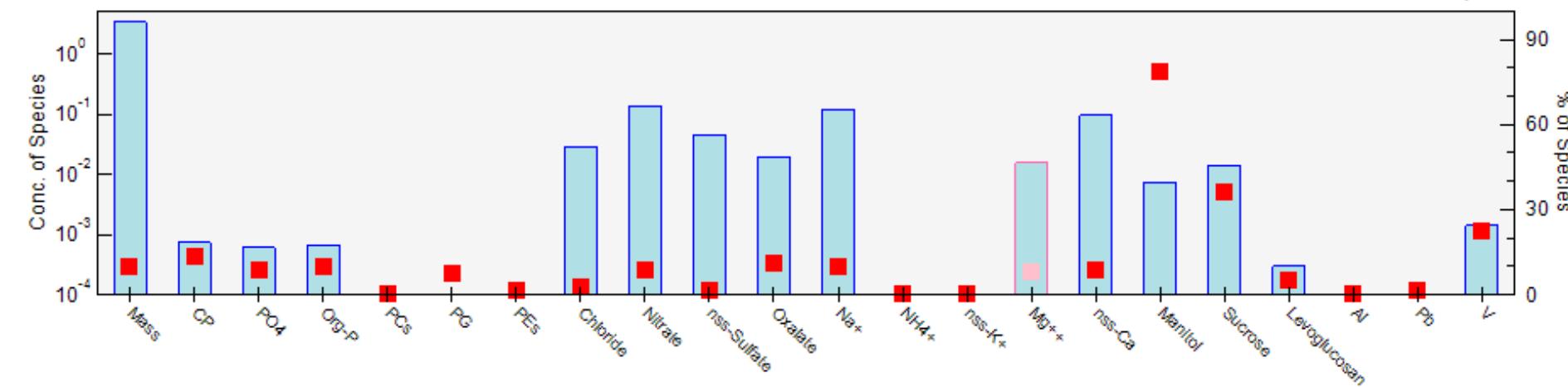
Dust



Cells
& Pollen

Factor Profile - Run 19 - Fungi

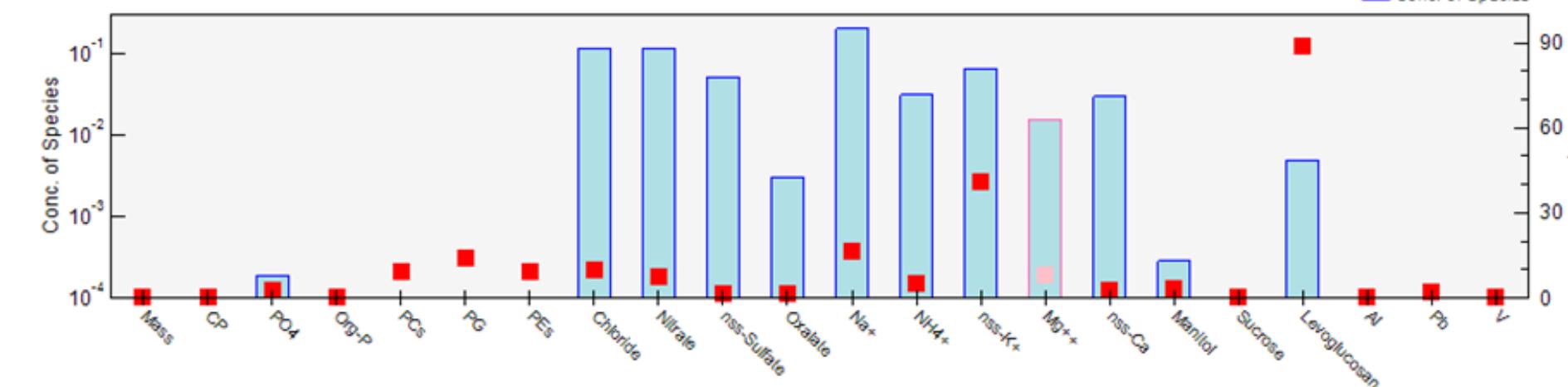
■ % of Species
■ Conc. of Species



Fungi

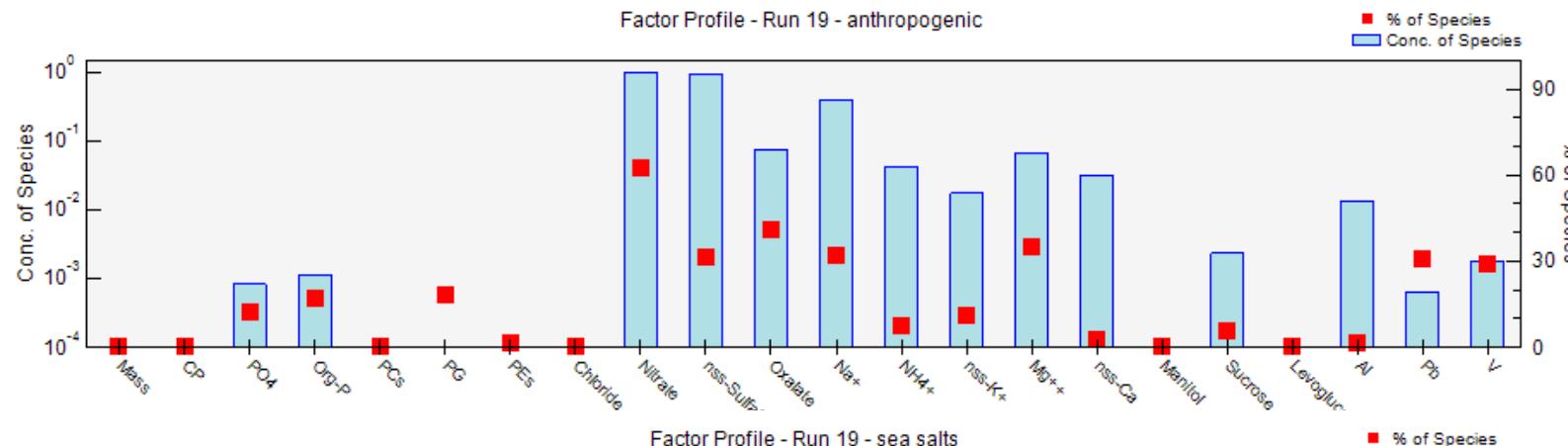
Factor Profile - Run 19 - BB

■ % of Species
■ Conc. of Species



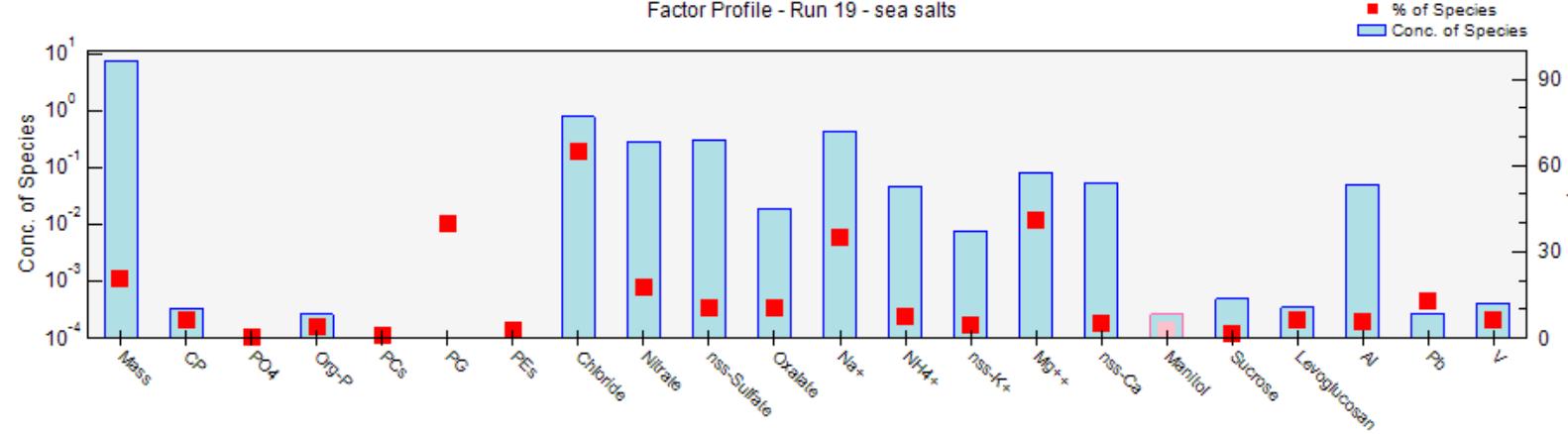
BB

Factor Profile - Run 19 - anthropogenic



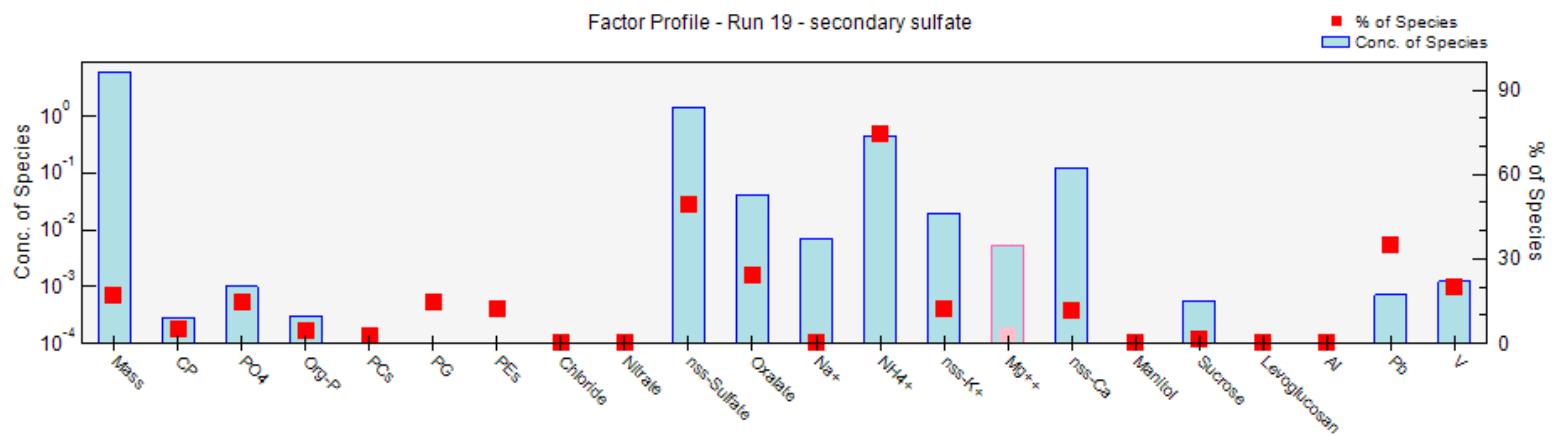
Anthropogenic

Factor Profile - Run 19 - sea salts



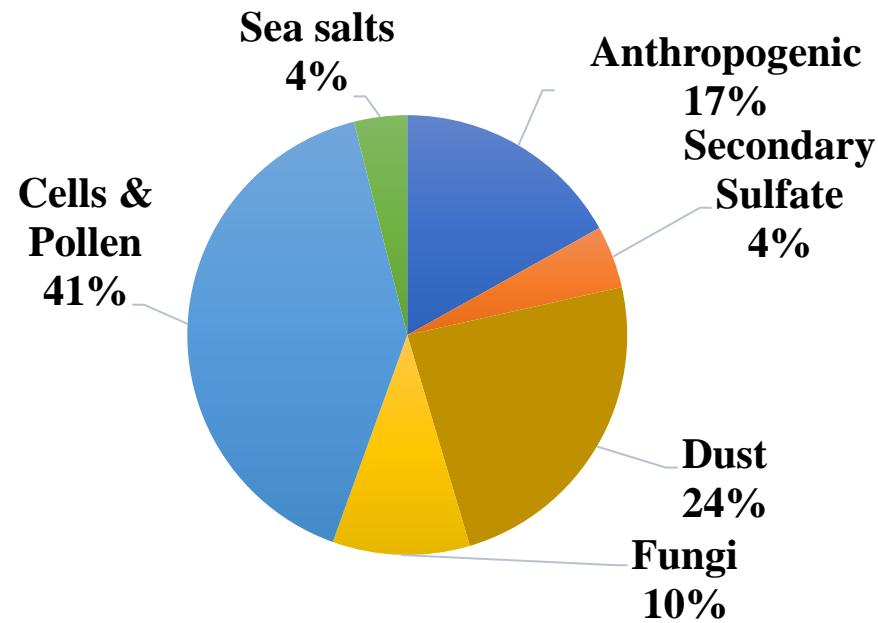
Sea salts

Factor Profile - Run 19 - secondary sulfate

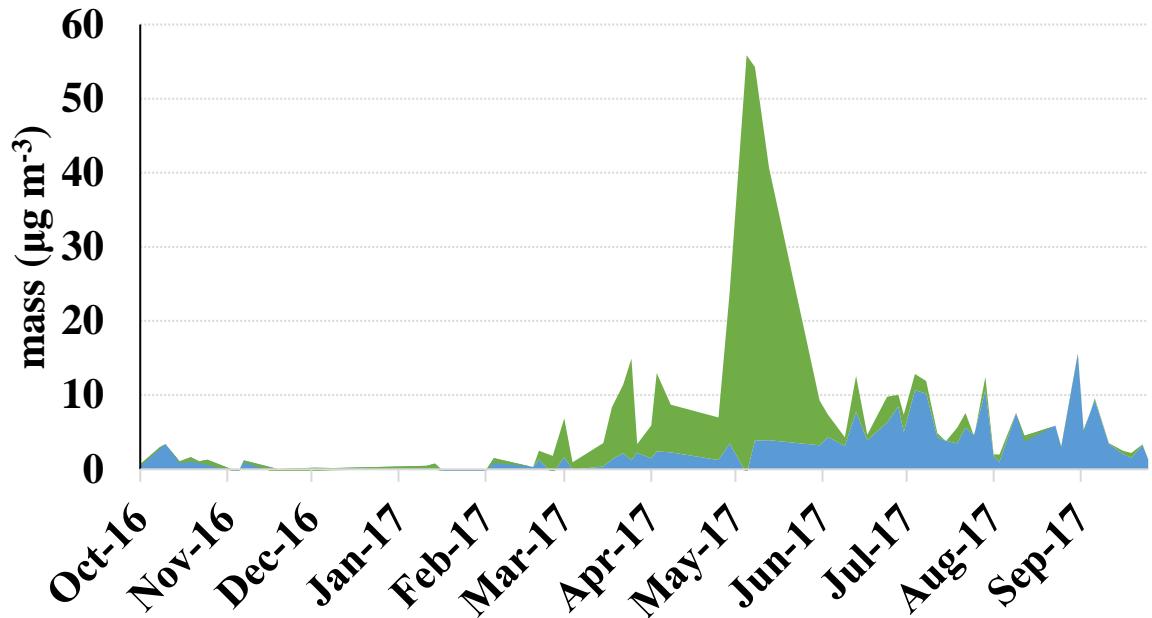


Secondary sulfate

Sources of organic P

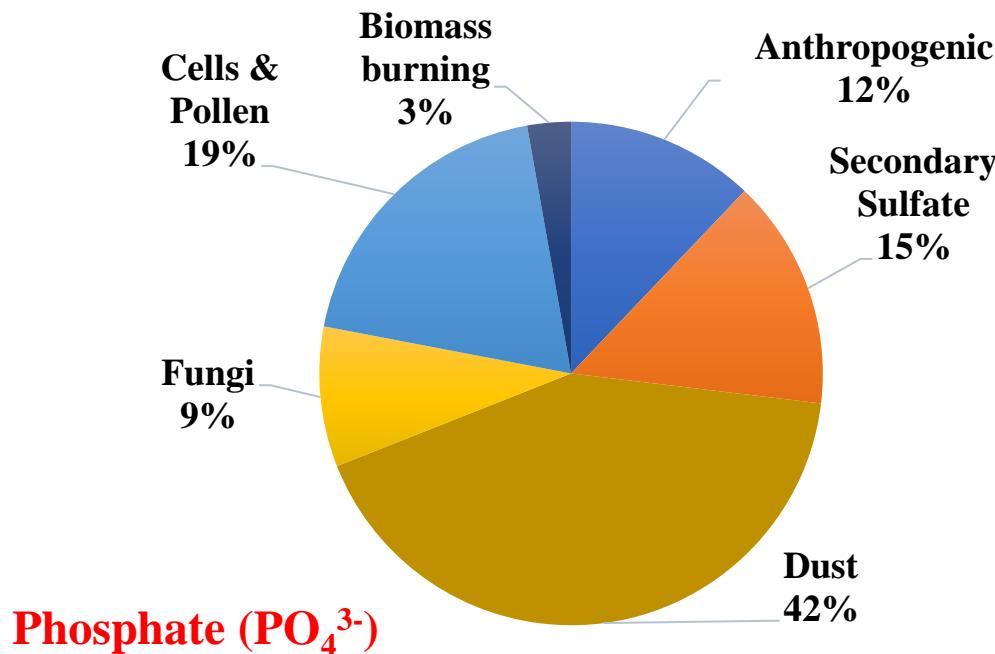


■ fungi ■ eukaryotic cells & pollen

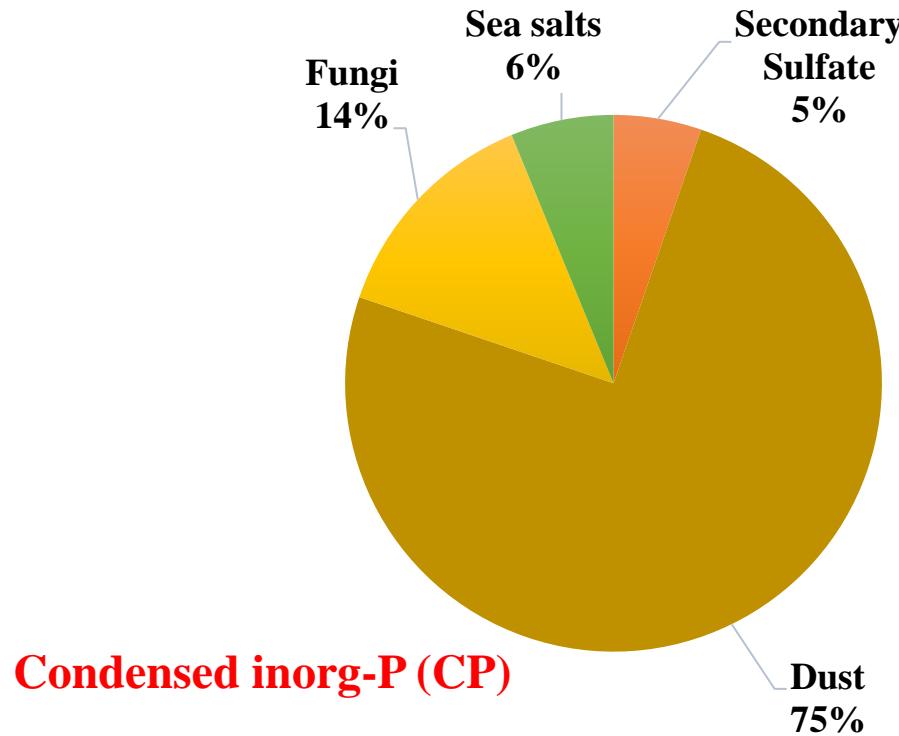


- Bioaerosols contribute with 51% to total org-P sources.
- They present seasonality, dominating during spring and summer (stratification period).
- Dust contribute with 24% to total org-P sources.
- The anthropogenic emissions are also important contributor to organic P fraction with ~17% and secondary produced due to acid solubilization is 4%. Global models suggest that 10% of atmospheric org-P is emitted from human activities (Kanakidou et al., 2012).

Sources of inorganic P



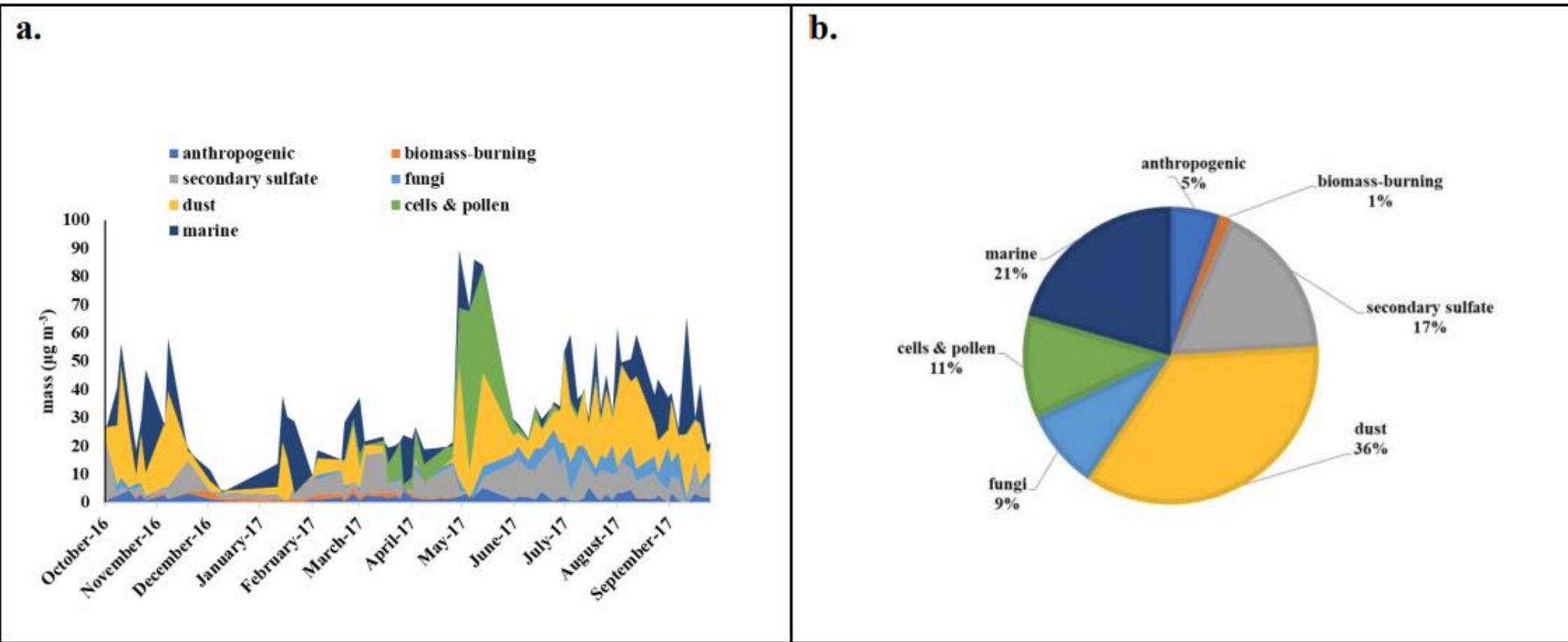
Phosphate (PO_4^{3-})



Condensed inorg-P (CP)

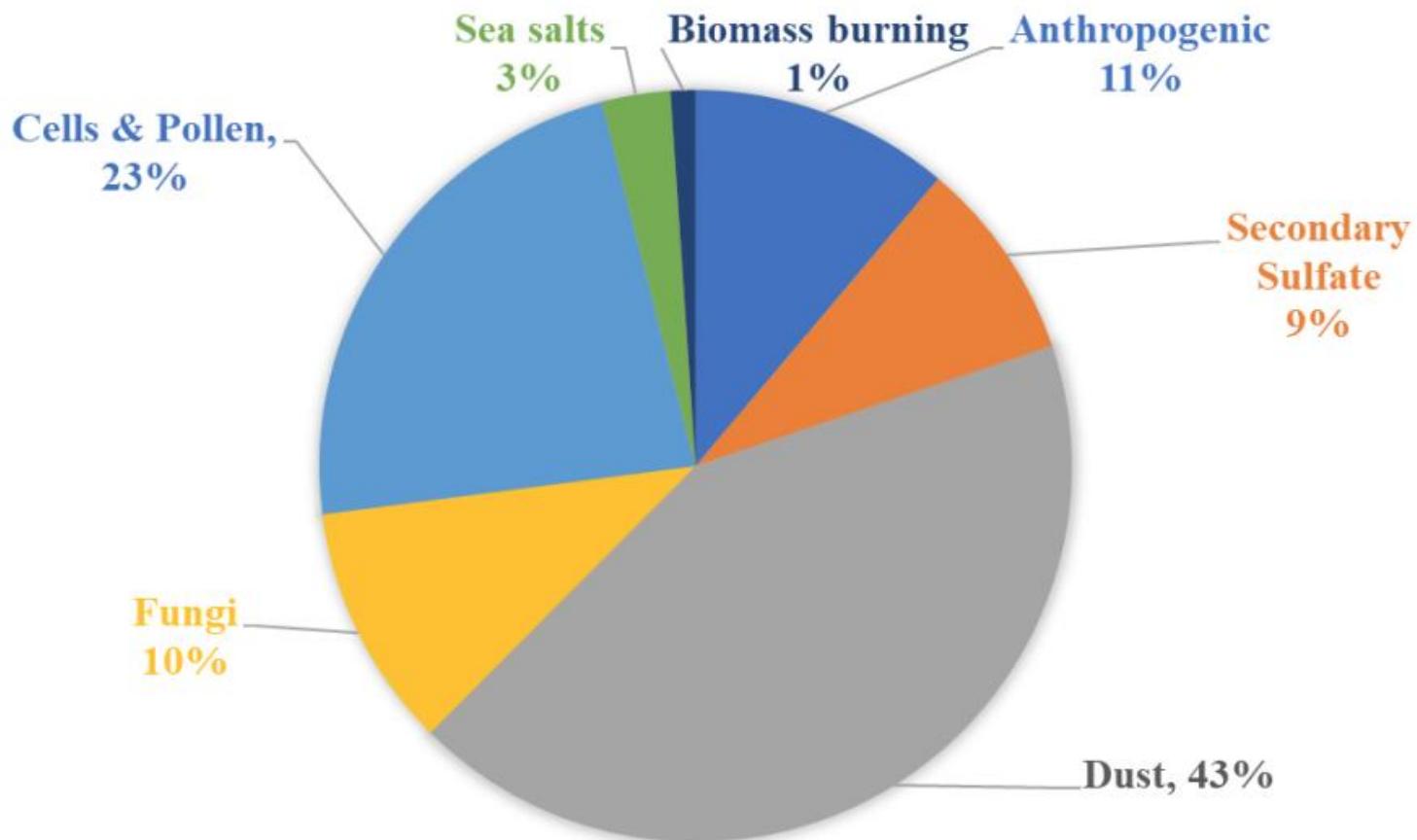
- Dust is the dominant source of both phosphate & CP.
- They present seasonality, dominating during spring and autumn.
- Anthropogenic emission produced more soluble P contributing primary with 12% and secondary with 15%. This estimation is similar with the proposed global percentage of 14.3% by Mahowald et al. (2008).

EXAMPLE-1



Supplementary Figure 6: Relative contributions to the particulate mass of the seven sources identified by PMF: contributions are shown with their variability in time (a) and expressed as average of the whole measurement period (b).

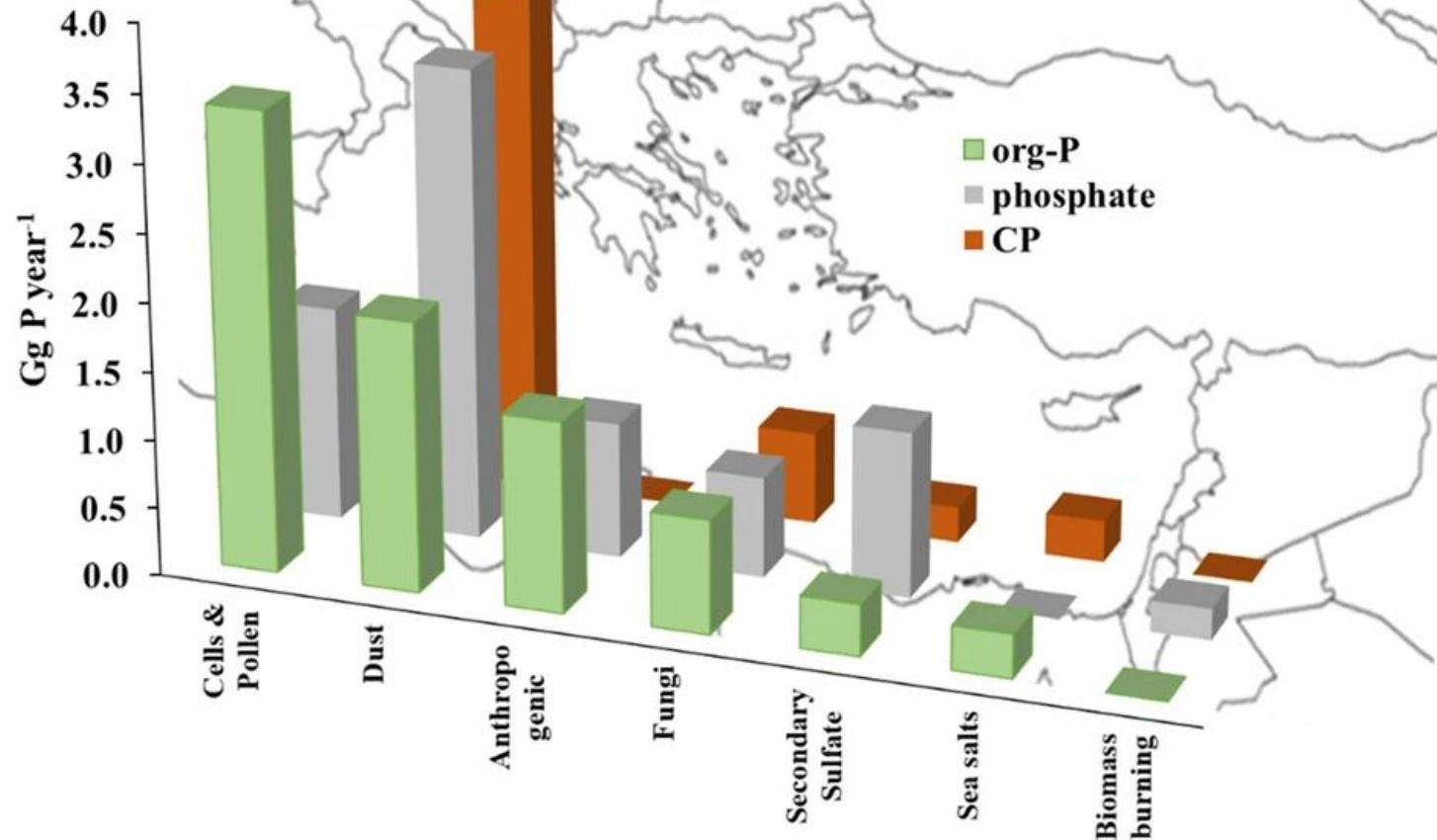
EXAMPLE-1



Supplementary Figure 8: Contribution percentage of the different atmospheric sources to total P (TP) over the Eastern Mediterranean area during a one-year period (2016-2017) for total suspended particles. TP was calculated to be 21.5 Gg P year⁻¹

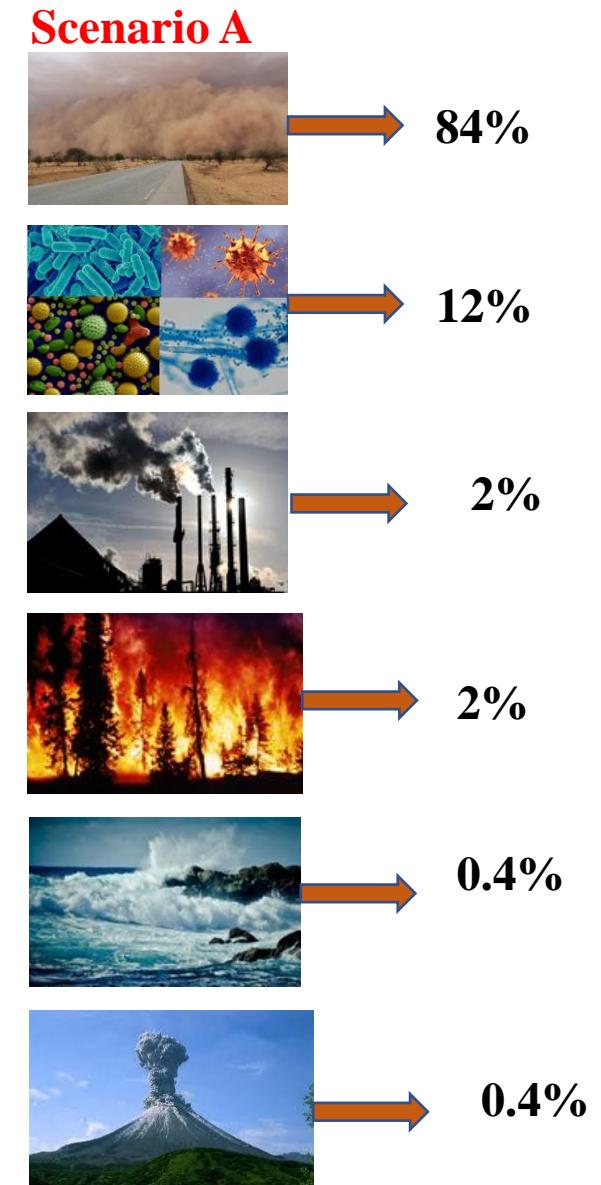
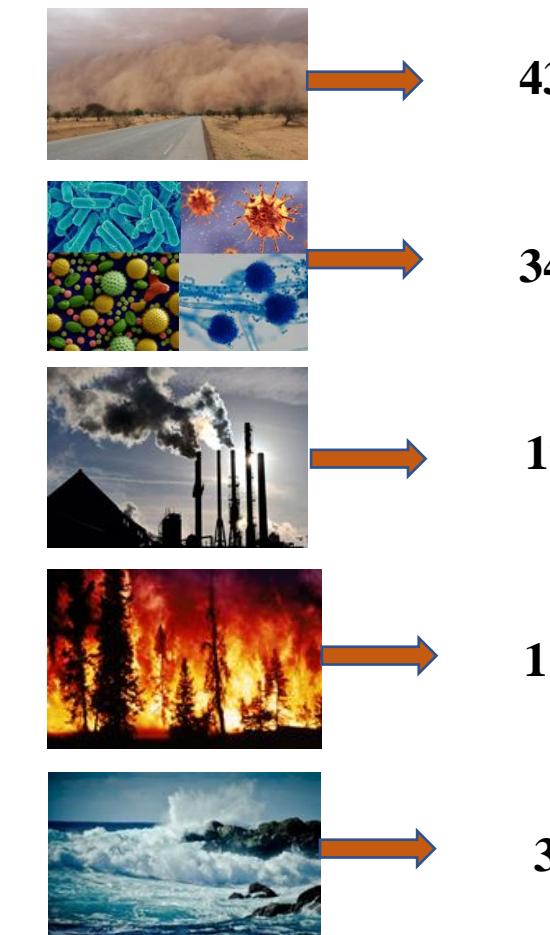
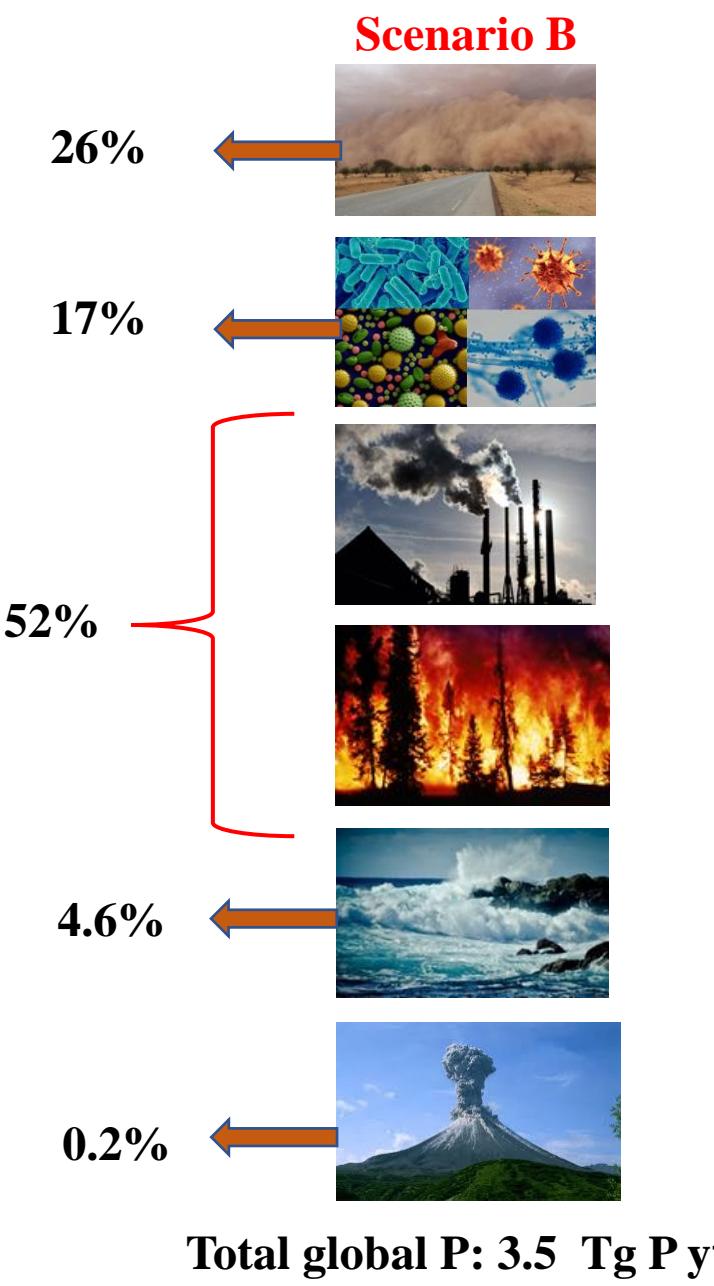
Bioaerosols and dust are the dominant sources of organic P in atmospheric particles

[Kalliopi Violaki](#) , [Athanasios Nenes](#), [Maria Tsagkaraki](#), [Marco Paglione](#), [Stéphanie Jacquet](#), [Richard Sempéré](#) & [Christos Panagiotopoulos](#)



Estimation of the annual deposition fluxes (in Gg P year^{-1}) of phosphorus species and their distribution to different sources over the eastern Mediterranean during one-year period (2016–2017) for total suspended particles. Total P was calculated to be $21.5 \text{ Gg P year}^{-1}$.

P sources over East Med.



Violaki et al., 2021

Mahowald et al., 2008, Myriokefalitakis et al., 2016

EXAMPLE-2

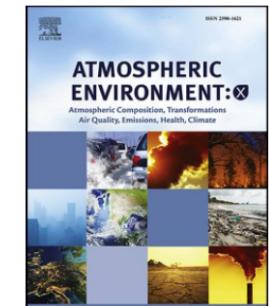
ATMOSPHERIC ENVIRONMENT: X 14 (2022) 100165



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Source identification of the elemental fraction of particulate matter using size segregated, highly time-resolved data and an optimized source apportionment approach

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^c MRC Centre for Environment and Health, Environmental Research Group, Imperial College London, UK

^d NIHR HPRU in Environmental Exposures and Health, Imperial College London, UK

^e Laboratory for Air Pollution and Environmental Technology, Swiss Federal Laboratories for Materials Science and Technology (Empa), Überlandstrasse 129, 8600, Dübendorf, Switzerland

EXAMPLE-2

Background of the study

This study aimed to:

- Identify the sources of PM elements in Zürich, Switzerland, using size-segregated elemental composition data.
- PMF analysis was performed using a combined dataset of $PM_{2.5}$ and PMcoarse ($PM_{10-2.5}$).
- The ***high-time resolution*** of the elemental data coupled with the size-segregated information led to improved Source Apportionment results in this urban environment.

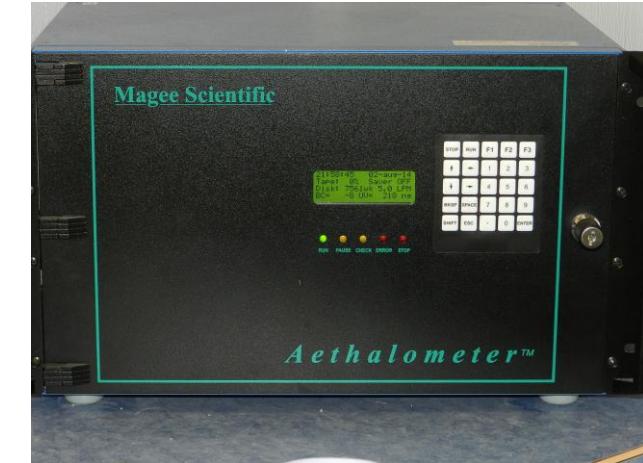


Fig. 1. The sampling point and central train station (right) in Zürich, Switzerland (left).

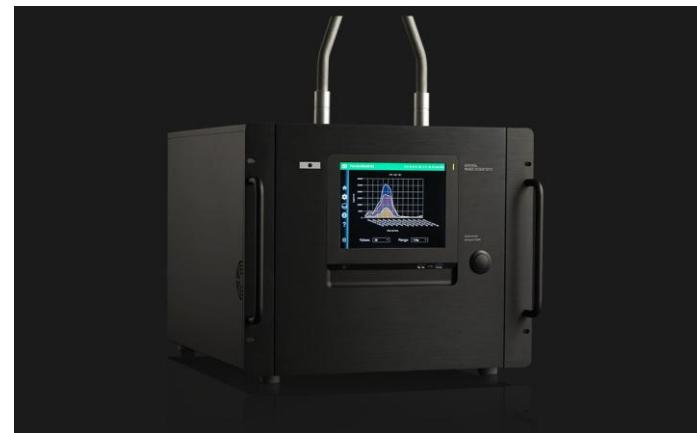
Instruments

- Q-ACSM \rightarrow Cl^- , NH_4^+ , NO_3^- , SO_4^{2-} , Organic Aerosols (OA)
- AE33 aethalometer \rightarrow Black Carbon
- Total carbon analyzer (TCA08) \rightarrow Total Carbon
- Xact 625i ambient metals monitor

$\text{PM}_{2.5}$ and PM_{10} concentrations of 37 elements (Al, Si, P, S, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Rb, Sr, Y, Zr, Nb, Cd, In, Sn, Sb, I, Ba, Hg, Tl, Pb, Bi)



Q-ACSM

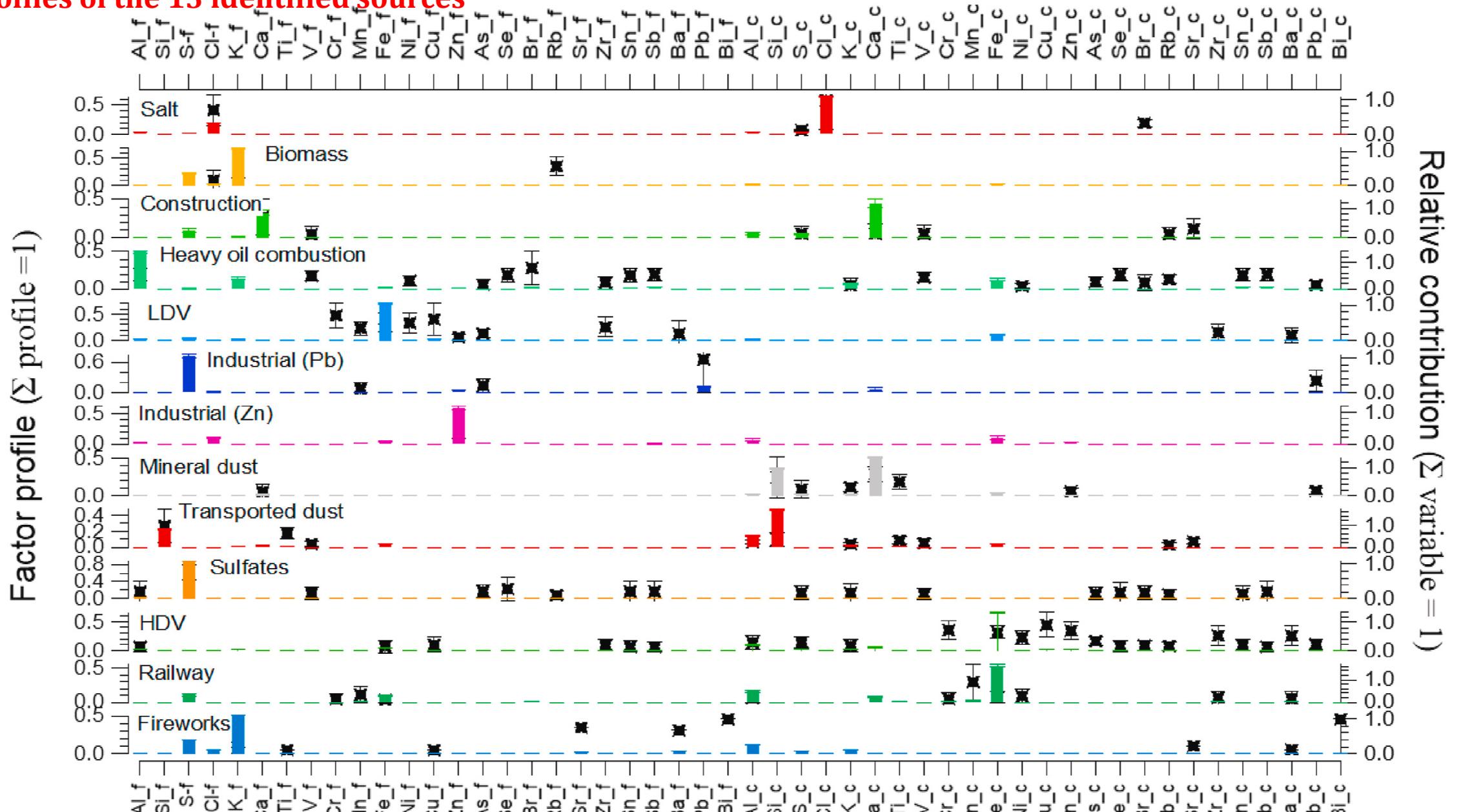


Total carbon analyzer



Xact 625i ambient metals monitor

Source profiles of the 13 identified sources



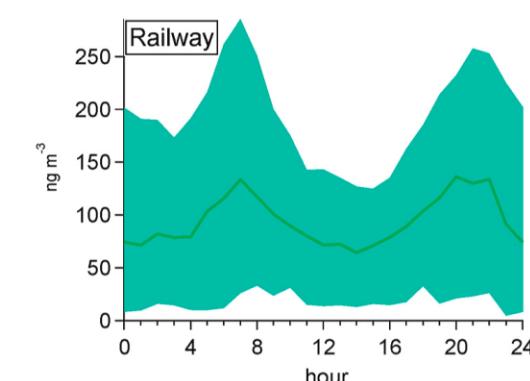
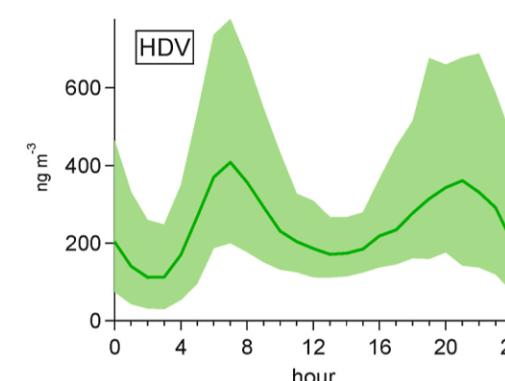
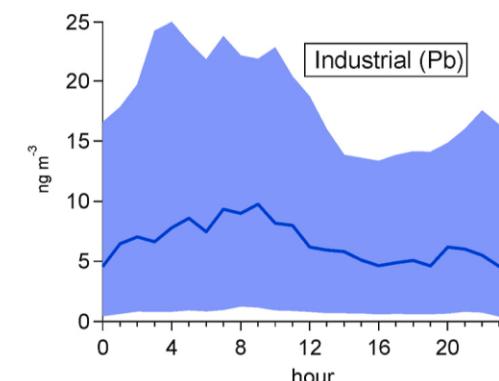
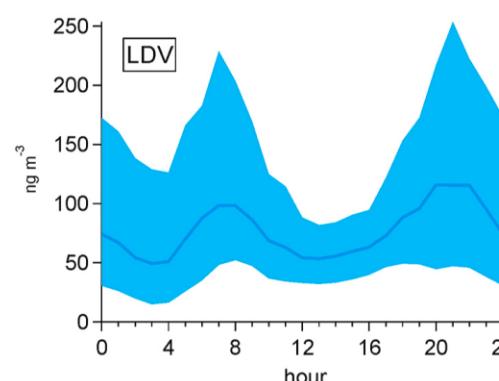
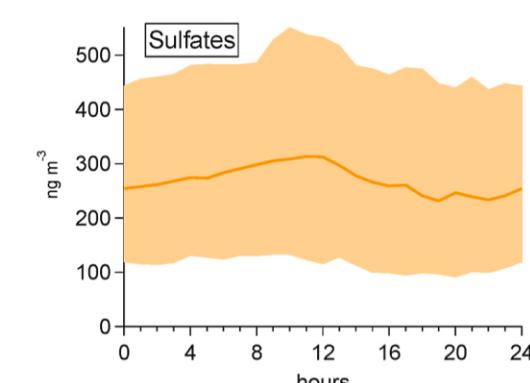
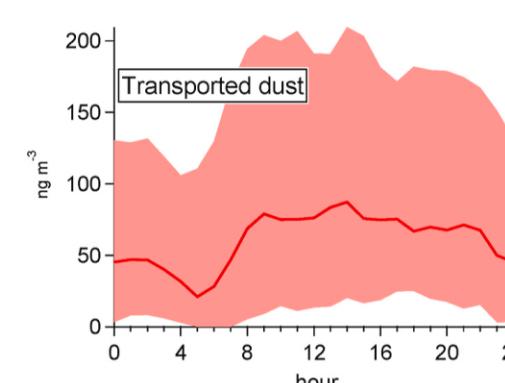
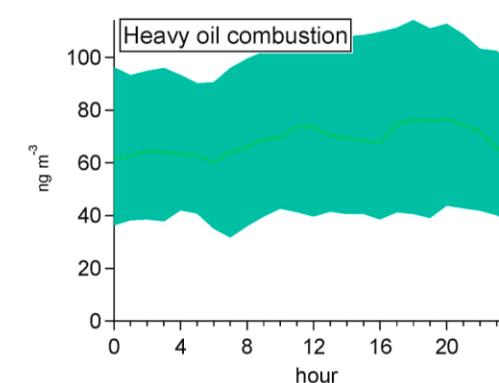
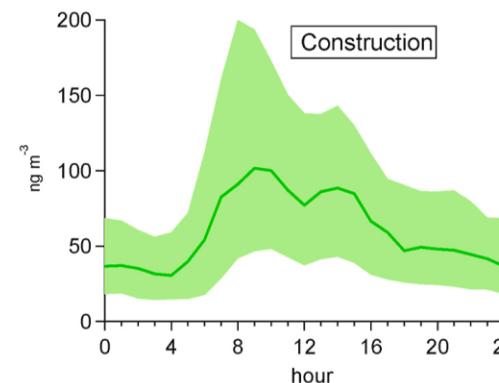
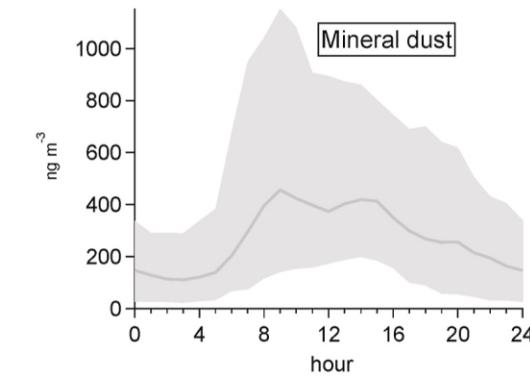
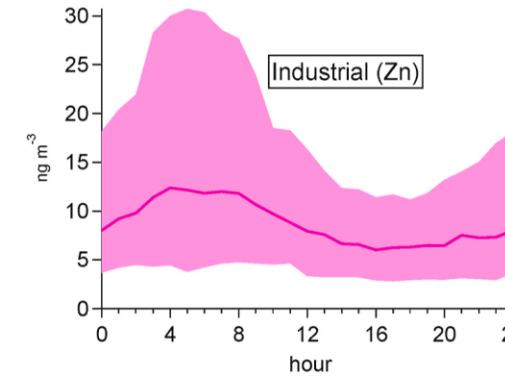
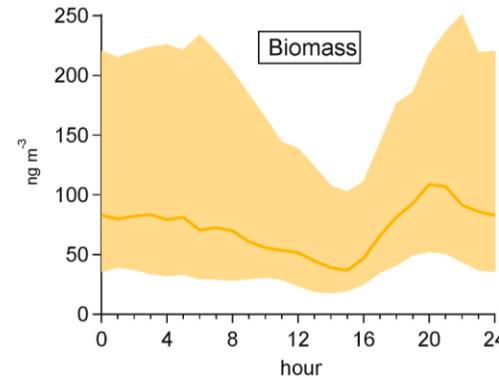
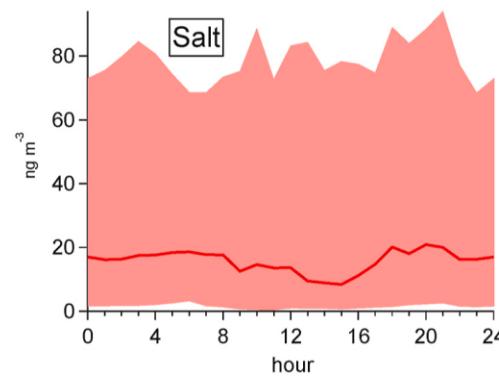
LDV: Light-Duty Vehicles

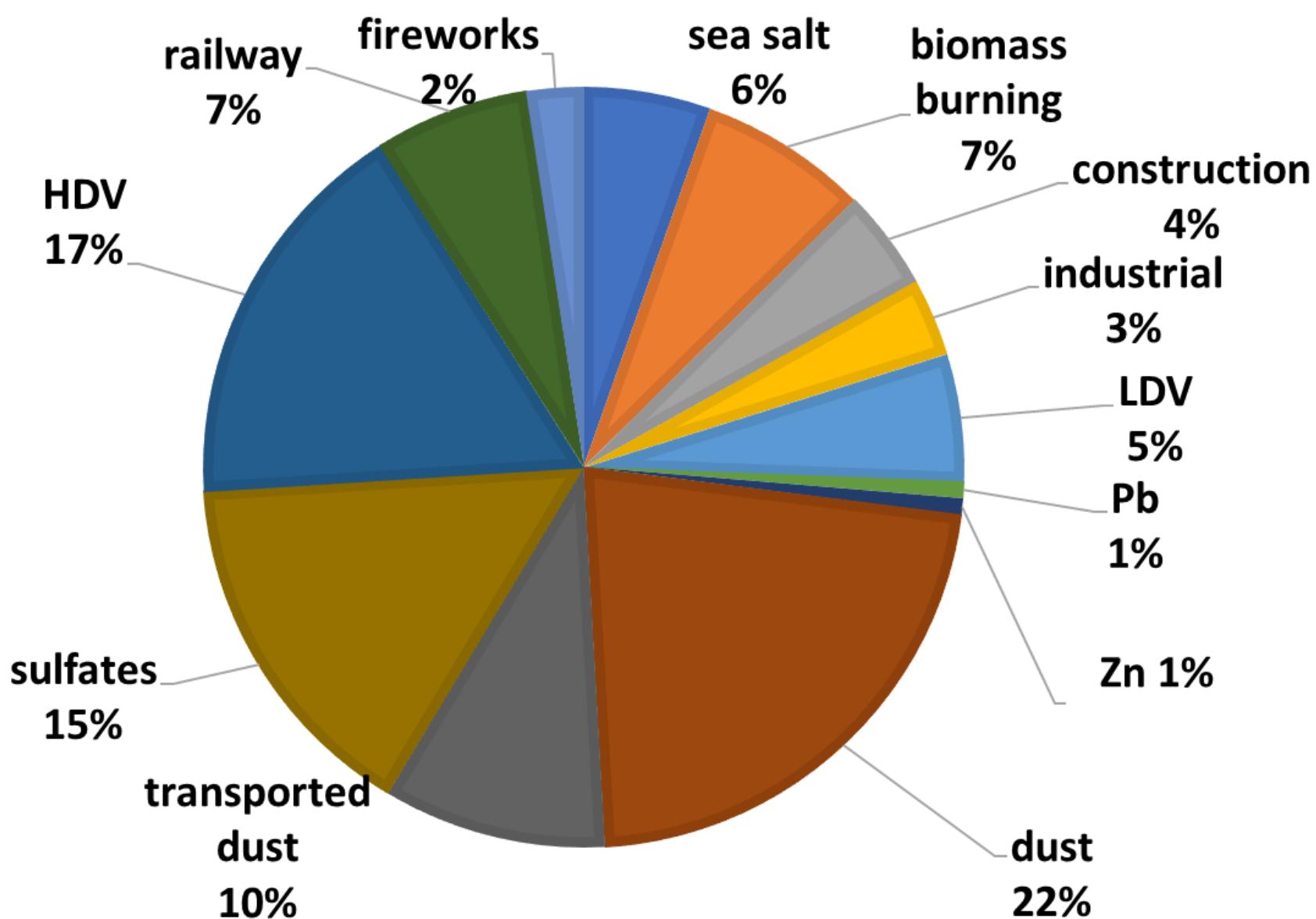
HDV: Heavy-Duty Vehicles

_c : coarse fraction

f the fine fraction

Median diurnal variation of the source contributions in ng m^{-3}





EXAMPLE-3

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Atmospheric
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Source apportionment of $\text{PM}_{2.5}$ in Montréal, Canada, and health risk assessment for potentially toxic elements

Nansi Fakhri^{1,2,4}, **Robin Stevens**^{2,3}, **Arnold Downey**², **Konstantina Oikonomou**⁴, **Jean Sciare**⁴,
Charbel Afif^{1,4}, and **Patrick L. Hayes**²

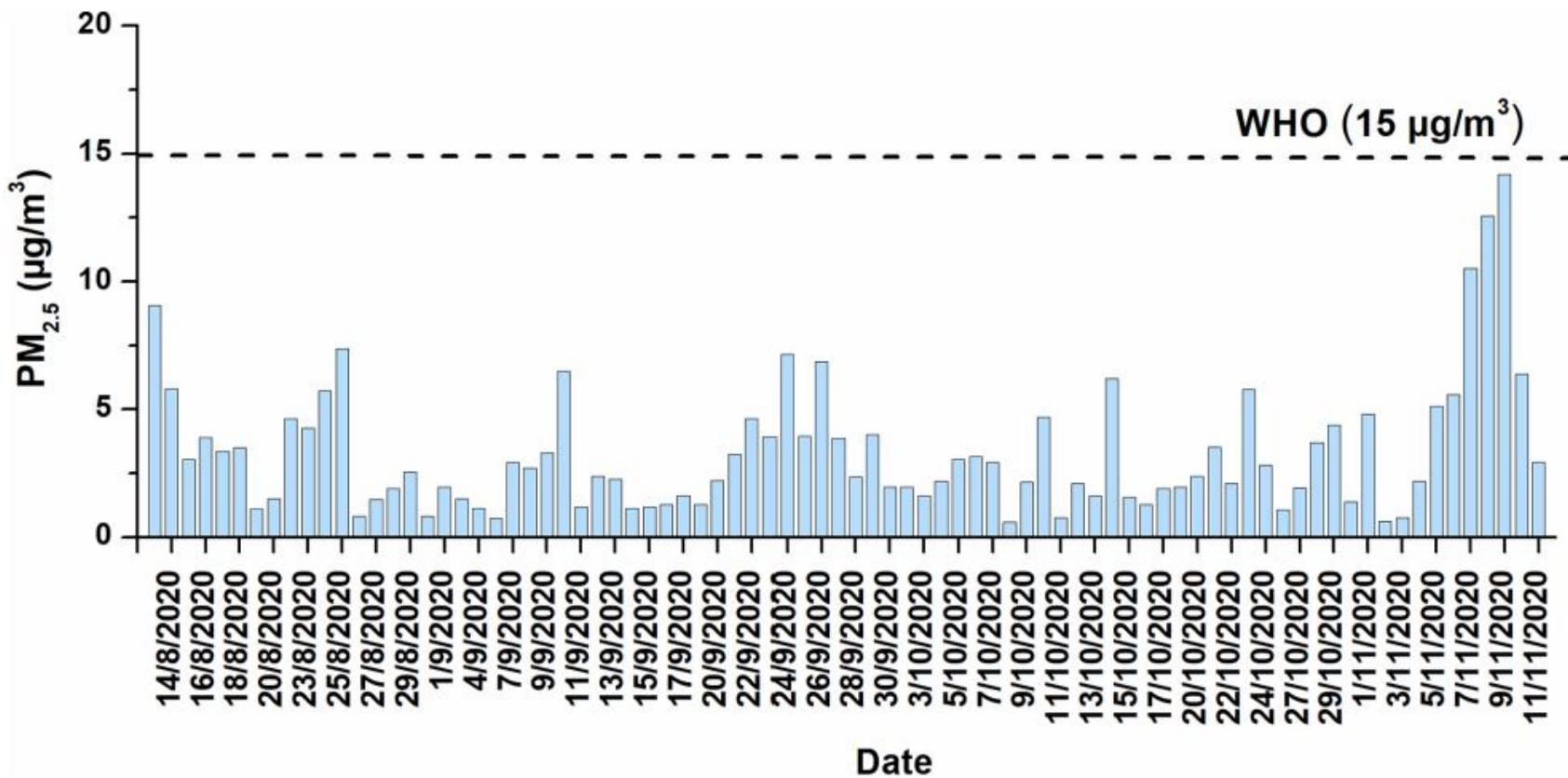


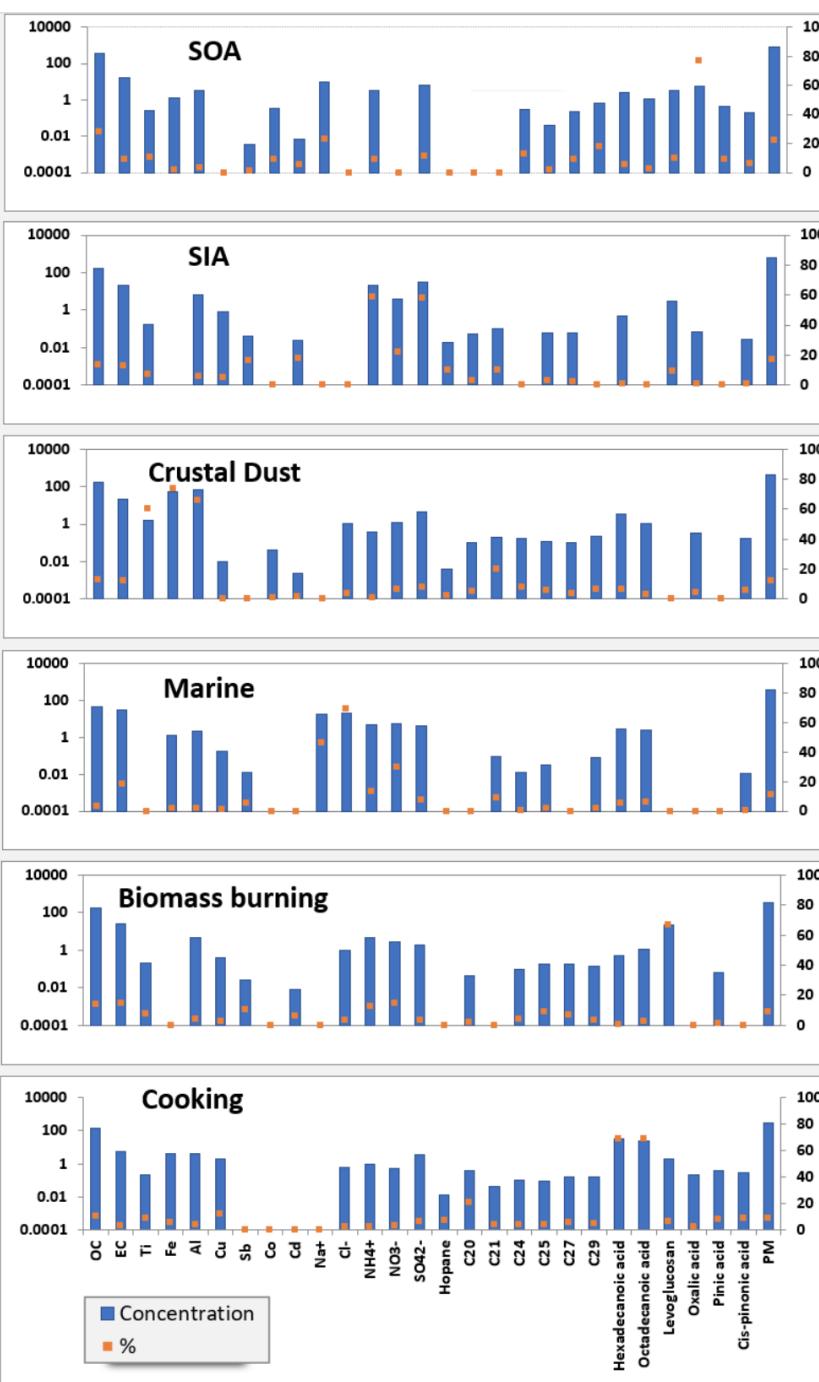
Figure 1. The temporal variation of PM_{2.5} concentrations for the sampling period (13 August to 11 November 2020).

Sampling was conducted at an urban site in Montréal from 13 August to 11 November 2020. The sampling site, labeled as MTL, was located on the rooftop of campus MIL (12 m above ground level) at the University of *Montréal* (45°31'02.100 N, 73°37'01.400 W) in the neighborhood of Outremont. The site is characterized by a *high density of residential and commercial premises*.

Average concentrations (ng m⁻³) of organic compounds in PM_{2.5}

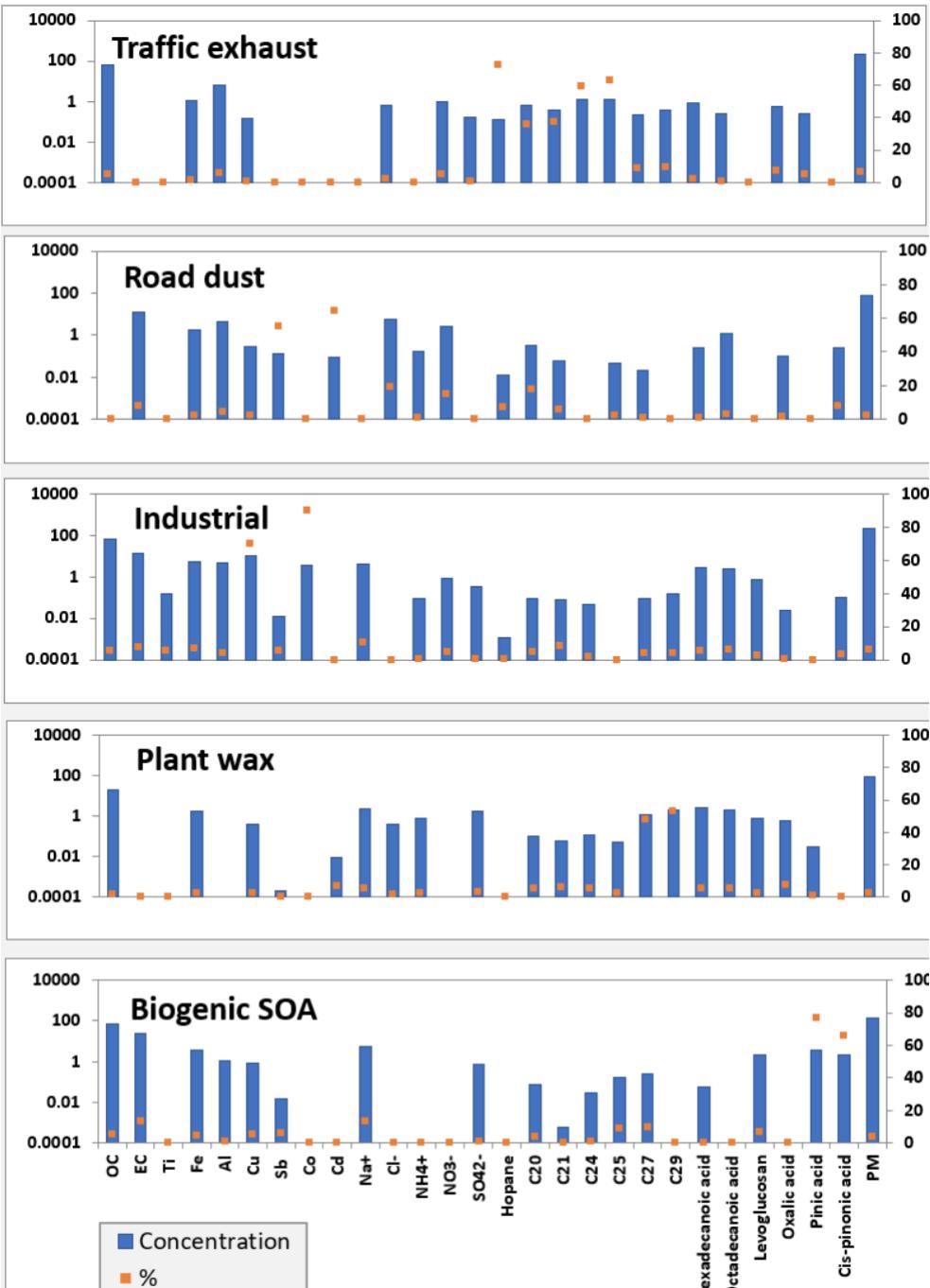
	Mean	SD	Range
17 α (H)-21 β (H)-Hopane	0.18	0.01	0.06–0.70
<i>n</i> -Alkanes			
Tetradecane (C14)	0.58	0.31	0.20–1.73
Pentadecane (C15)	0.48	0.66	0.28–4.27
Hexadecane (C16)	0.75	0.37	0.34–2.04
Heptadecane (C17)	0.71	0.67	0.22–5.20
Octadecane (C18)	0.99	1.69	0.18–8.29
Nonadecane (C19)	0.46	0.24	0.17–1.26
Eicosane (C20)	1.82	1.20	0.73–7.90
Heneicosane (C21)	0.99	0.35	0.37–2.14
Docosane (C22)	0.96	1.15	0.37–8.49
Tricosane (C23)	1.02	0.42	0.40–2.16
Tetracosane (C24)	2.24	1.61	0.82–11.16
Pentacosane (C25)	1.97	1.02	0.83–4.97
Hexacosane (C26)	1.51	0.84	0.48–3.96
Heptacosane (C27)	2.52	2.89	0.74–23.82
Octacosane (C28)	1.79	2.84	0.45–23.20
Nonacosane (C29)	3.84	3.78	0.73–3.37
Triacontane (C30)	1.12	1.41	0.12–7.07
Hentriacontane (C31)	1.56	0.96	0.34–6.72

Sugars				
Levoglucosan	33.72	6.45	6.45–126.40	
Mannosan	1.03	0.94	0.15–4.59	
Mannitol	2.14	3.22	0.23–18.91	
Arabitol	3.14	4.29	0.29–39.00	
Glucose	2.92	3.01	0.17–24.47	
Fatty acids				
Tetradecanoic acid	4.17	1.40	1.66–7.97	
Hexadecanoic acid	51.12	13.09	28.39–87.43	
Octadecanoic acid	37.06	9.41	18.05–64.90	
Oleic acid	4.43	1.65	2.51–13.05	
Dicarboxylic acids (DCAs)				
Oxalic acid (diC2)	7.79	1.58	0.28–15.03	
Adipic acid(diC6)	1.60	4.18	0.31–3.42	
Azelaic acid (diC9)	5.93	2.18	1.12–15.01	
Biogenic SOA tracers				
Pinic acid	4.73	1.78	0.21–8.93	
<i>cis</i> -Pinonic acid	3.17	1.71	0.62–9.73	



Secondary inorganic aerosol (SIA) factor

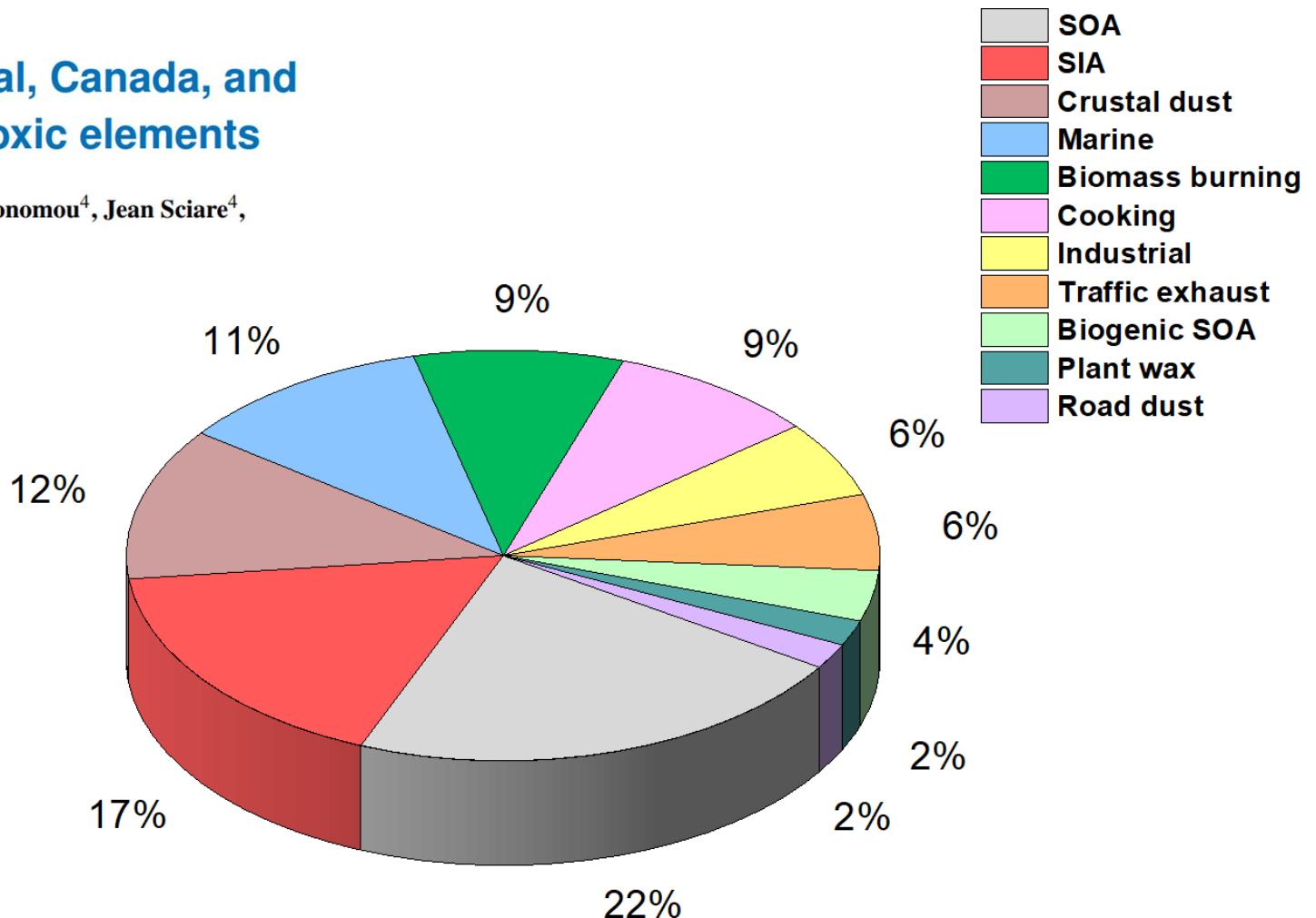
Eleven factors



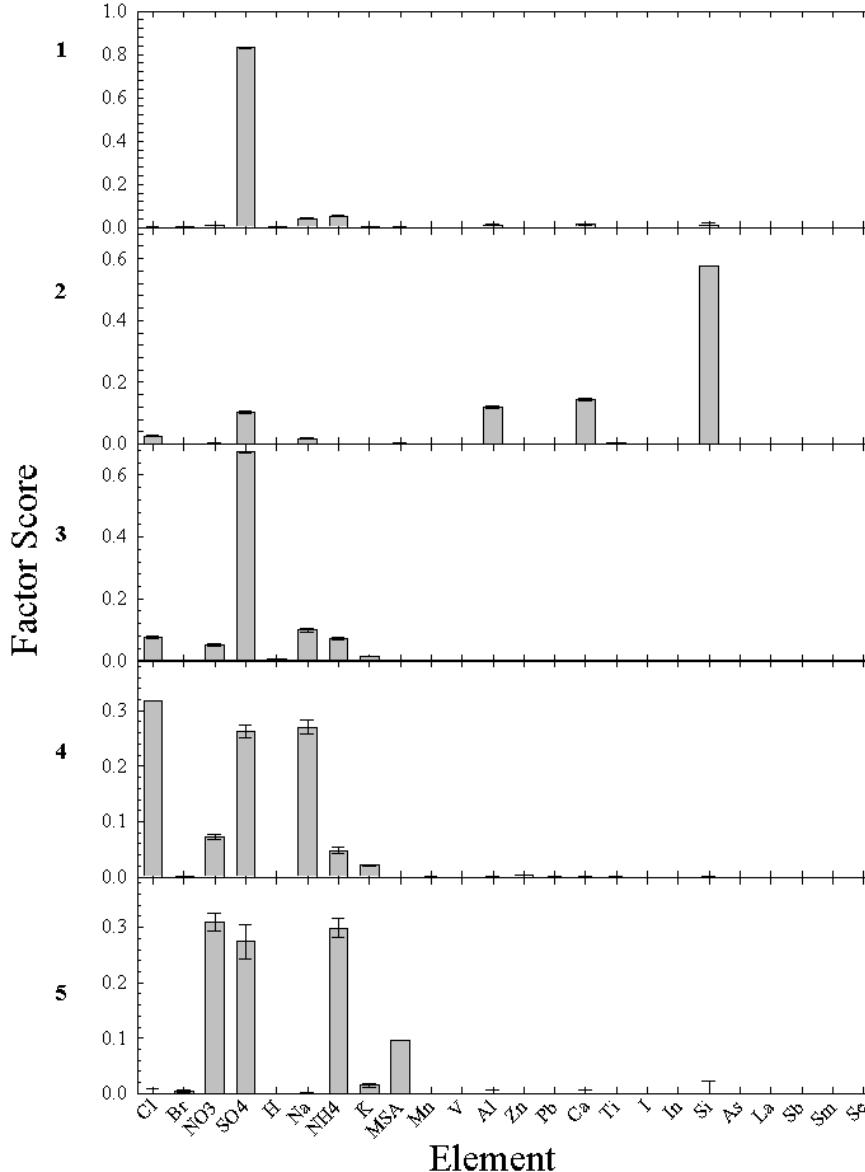


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ARCTIC HAZE



Photochemistry at
Polar Sunrise

Soil

Transported
Sulfate

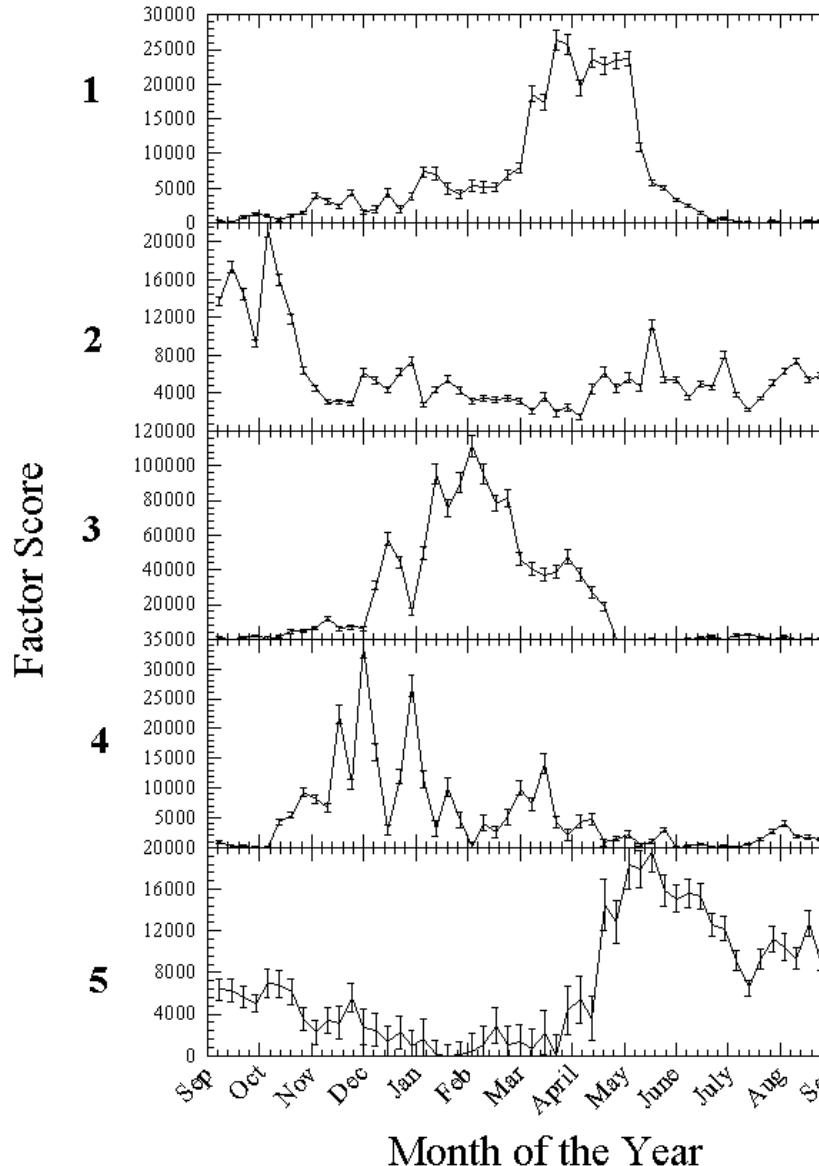
Sea Salt

Biogenic sulfate

Credit to Prof. Hopke



ARCTIC HAZE



Credit to Prof. Hopke

Photochemistry at Polar
Sunrise

Soil

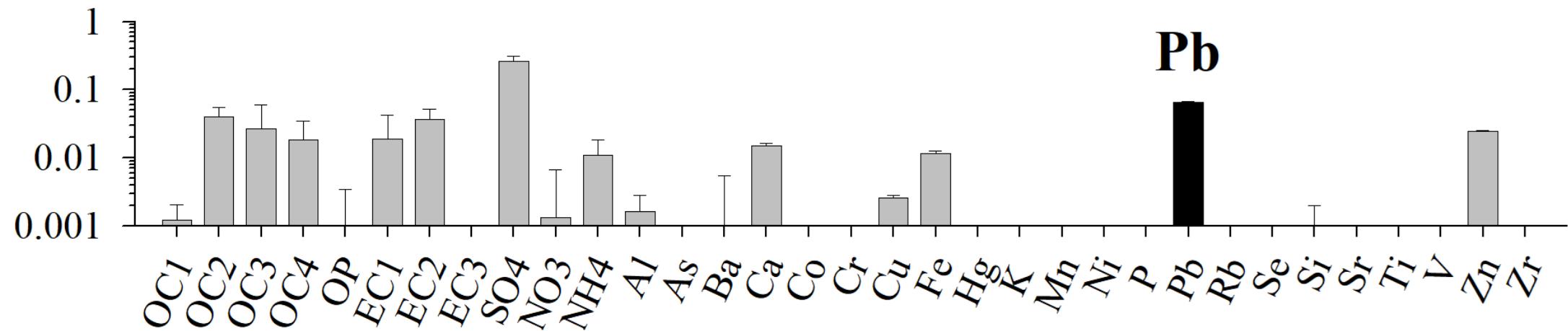
Transported
Sulfate

Sea Salt

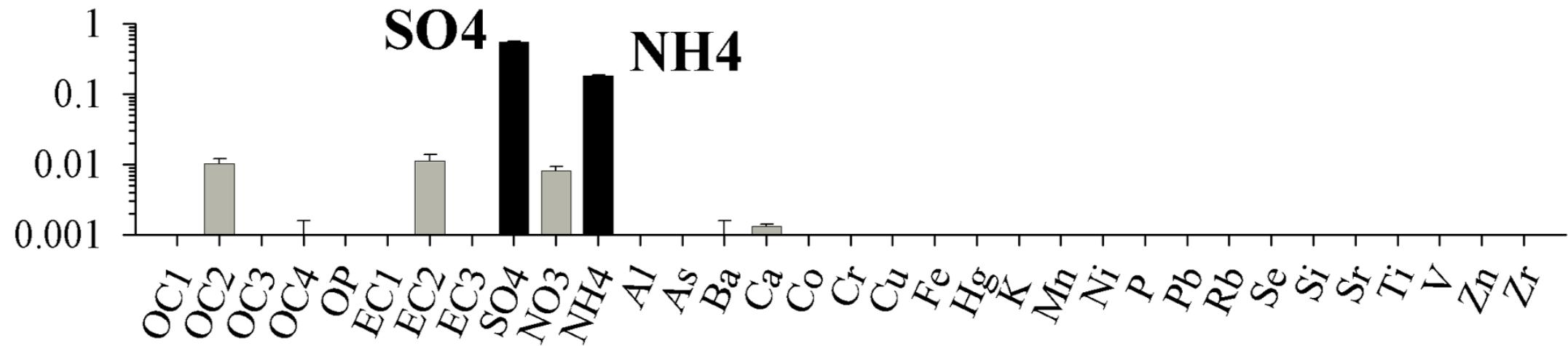
Biogenic sulfate



Lead Smelting



Secondary Sulfate



Thank You

Questions?

e-mail: kalliopi.violaki@epfl.ch