

Supplementary Material: A holistic approach based on bio-monitoring techniques and satellite observations for air pollution assessment and health risk impact of atmospheric trace elements in a semirural area of Southern Italy (High Sauro Valley)

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Supplementary S1: Human health exposure assessment

The carcinogenic risk posed to the exposure of Cd, Cr(VI), Ni and Pb contained in the atmospheric aerosol particles through inhalation and the non-carcinogenic effect posed by Cd, Cr(VI) Cu, Mn, Ni, Pb and Zn through ingestion, dermal contact and inhalation pathways were evaluated using the model developed by the United States Environmental Protection Agency [49] The carcinogenic and non-carcinogenic health risk was assessed for both children and adults. The chemical daily intake (CDI), dermal absorbed dose (DAD), exposure concentration (EC) was estimated by the following equations [50]:

$$CDI_{ingest} = \frac{C \times IngR}{BW} \times \frac{EF \times ED}{AT} \times CF \quad (1)$$

$$DAD_{dermal} = \frac{C \times SA \times AF \times ABS}{BW} \times \frac{EF \times ED}{AT} \times CF \quad (2)$$

$$EC_{inh} = C \times \frac{ET \times EF \times ED}{ATn} \quad (3)$$

where: C is metal concentrations in the sampler (mg/Kg); IngR: ingestion rate (according to US EPA model, the default values for the ingestion exposure of soil/dust were 200 mg/day for children and 100 mg/day for adults); EF: exposure frequency (250 days year⁻¹); ED: exposure duration (6 years for children and 24 years for adults); BW: the average body weight (15 kg for children and 70 kg for adults); AT: averaging time (for non-carcinogens, AT = ED

x365 days; for carcinogens, $AT = 70 \times 365 = 25,550$ days); CF: conversion factor (10^{-6} kg mg^{-1}); SA: surface area of the skin that contacts the airborne particulates (3300 cm² for adults and 2800 cm² for children); AF: skin adherence factor for the airborne particulates (0.2 mg/cm² for both adults and children); ABS: dermal absorption factor (0.001) for Cd; no values were available for other elements; therefore, a conservative value of 1.0% was used in the present study (ICMM, 2007); ET: exposure time (hours/day); ATn: average time (for non-carcinogens, $AT = ED \times 365$ days \times 24 hours/day; for carcinogens, $ATn = 70$ year \times 365 days/year \times 24 h). All parameters used in the calculation of CDI, DAD and EC were reported in US EPA, [51].

The possible carcinogenic effect of Cd, Cr (VI), Ni and Pb contained aerosol particles was considered by excess lifetime cancer risk (ELCR) and calculated according to the formula reported in the literatures [52] as follows:

$$ELCR = EC \times IUR \quad (4)$$

Where EC is the exposure concentration and IUR is the inhalation unit risk ($\mu g / m^3$)⁻¹. The integrated excess lifetime cancer risk was also determinate as the sum of ELCR values ($\Sigma ELCR$) for the considered carcinogenic elements. USEPA considers that if the ELCR values are less than 1×10^{-6} , (about 1 out of a 1,000,000 change) the risk arising from carcinogens could be negligible, for ELCR values between 1×10^{-6} and 1×10^{-4} some sort of remediation is desirable while for ELCR greater than 1×10^{-4} , it was indicated that the potential risk of cancer is posed seriously. [51,53]

The non-carcinogenic risk was evaluated by the hazard quotient (HQ) and hazard index (HI). HQ posed by Cd, Cr(VI), Cu, Mn, Ni, Pb and Zn contents atmospheric aerosol through ingestion (HQ_{ing}), dermal contact (HQ_{derm}) and inhalation (HQ_{inh}) pathway were calculated as follows:

$$HQ_{ing} = \frac{CDI_{ing}}{RfDo} \quad (5)$$

$$HQ_{derm} = \frac{DAD_{derm}}{RfDo} \quad (6)$$

$$HQ_{inh} = \frac{EC_{inh}}{RfCi \times 1000 \mu g / mg} \quad (7)$$

$$HI = \sum HQ_i \quad (8)$$

where HQ_i is the hazard quotient of the i -th element, $RfDo$ is the oral reference dose ($mg \text{ Kg}^{-1} \text{ day}^{-1}$); $RfCi$ is the inhalation reference concentrations (mgm^{-3}). Integrated HI correspond to the sum of the single HQ_i calculated for each element considered and was calculated as Eq. (8):

Values of HQ and/or HI greater than 1 indicate that non- carcinogenic effects may happened. The greater the HQ and/or HI value, the higher the probability of non- carcinogenic effects [51].

Table S1 Experimental values (mean value±standard deviation) and certified values are referred to the International Atomic Energy Agency (IAEA) standard reference material, IAEA 336. Recovery percentage and method detection limit (MDL) results were also reported.

Elements	Experimental value (mg kg ⁻¹)	Certified values (mg kg ⁻¹)	Recovery (%)	MDL (ppm)
Al ^(a)	482±71	680	71	0.04665
Ca ^(a)	-	not reported	-	0.20283
Cd ^(b)	0.155±0.12	0.117	133	0.00152
Cr ^(a)	1.265±0.20	1.060	119	0.00324
Cu ^(b)	4.952±1.16	3.600	138	0.00865
Fe ^(a)	361±6	430	84	0.13140
K ^(a)	1734±41	1840	94	0.00867
Li ^(a)	-	not reported	-	0.00006
Mg ^(a)	-	not reported	-	0.00423
Mn ^(a)	48±2	63	76	0.06187
Na ^(a)	310±24	320	97	0.03230
Ni ^(a)	-	not reported	-	0.00354
P ^(a)	522±27	610	86	0.00415
S ^(a)	-	not reported	-	8.16875
Pb ^(b)	4.919±0.98	4.900	105	0.08070
Ti ^(a)	-	not reported	-	0.01488
Zn ^(a)	31±3	30.4	103	0.00282

^a ICP-OES

^b GF-AAS

Table S2. Spectral and spatial characterization of the Landsat 8 OLI-TIRS bands.

Number of Band	Band Width (μm)	Band Description	Spatial Resolution (m)
1	0.435–0.451	Coastal aerosol	30
2	0.452–0.512	Blue	30
3	0.533–0.590	Green	30
4	0.636–0.673	Red	30
5	0.851–0.879	Near infrared (NIR)	30
6	1.566–1.651	Short wavelength infrared (SWIR) 1	30
7	2.107–2.294	SWIR 2	30
8	0.503–0.676	Panchromatic	15
9	1.363–1.384	Cirrus	30
10	10.60–11.19	Thermal infrared sensor (TIRS)	100
11	11.50–12.51	TIRS 2	100

Table S3. Mean value \pm standard deviation ($m \pm sd$), contamination Factor (CF) and Igeo indexes of the trace element concentrations measured in the lichen bags after 1-month exposure. The mean values of the trace element concentrations are highlighted in bold.

Trace element concentrations	1-month exposure	CF
Al	1480 \pm 493	1.3
Ca	27186 \pm 7822	1.4
Cd	0.7 \pm 0.2	1.4
Cr	2.1 \pm 0.7	1.1
Cu	5 \pm 2	1.3
Fe	1070 \pm 303	1.1
K	6709 \pm 1038	1.1
Li	2 \pm 0.1	1.3
Mg	1741 \pm 274	1.4
Mn	148 \pm 36	1.1
Na	506 \pm 300	1.9
Ni	4 \pm 1	1.1
P	971 \pm 189	1.2
Pb	18 \pm 8	1.1
S	1943 \pm 238	1.1
Ti	31 \pm 9	1.2
Zn	83 \pm 17	0.9

Table S4. Contamination factors (CF). pollution load indexes (PLI) calculated using lichen bags and NDVI' values for the 23 monitoring samples

Monitoring samples	CF																	PLI	NDVI'
	Al	Ca	Cd	Cr	Cu	Fe	Li	K	Mg	Mn	Na	Ni	P	Pb	S	Ti	Zn		
1	0.8	1.0	1.2	1.1	1.1	0.9	1.0	1.0	1.0	0.9	1.2	0.9	1.1	1.5	1.1	0.9	1.1	1.1	0.003
2	1.0	1.7	1.2	0.9	1.5	1.2	1.0	1.4	1.3	1.1	1.5	1.3	1.2	1.5	1.0	0.8	1.4	1.2	0.545
3	0.9	0.9	0.9	0.9	1.0	1.0	1.2	1.2	1.2	1.2	1.1	0.7	1.2	0.8	1.1	1.2	0.9	1.0	0.228
4	0.8	1.3	1.5	0.6	1.2	0.7	1.1	1.1	1.1	0.9	1.5	0.7	1.0	1.0	1.0	1.0	0.8	1.0	0.241
5	1.4	1.9	1.3	0.9	0.9	0.9	1.2	1.2	1.3	1.0	1.8	1.1	1.0	0.6	0.9	1.4	0.7	1.1	1.120
6	1.5	1.3	1.4	1.3	1.4	1.2	1.1	1.4	1.5	0.9	2.1	1.2	1.2	1.1	1.2	1.5	1.0	1.3	0.116
7	1.0	0.8	0.9	0.9	1.0	1.0	1.1	1.3	1.5	0.9	2.3	0.8	1.6	0.7	1.0	1.0	0.8	1.1	2.144
8	1.6	1.2	1.5	1.8	1.8	1.8	1.2	1.3	1.3	1.0	1.5	2.0	1.4	2.3	1.4	1.2	1.3	1.5	0.692
9	1.8	1.6	1.5	1.6	1.3	1.5	1.2	1.4	1.7	1.3	1.7	1.4	1.1	1.2	1.2	1.5	1.1	1.4	1.333
10	1.0	1.9	1.3	0.8	1.1	1.1	1.0	1.3	1.6	1.2	3.7	1.2	1.4	1.3	1.1	0.8	0.9	1.2	0.129
11	1.4	2.1	1.6	1.4	1.1	1.4	1.2	1.2	1.5	1.2	1.8	1.4	1.1	1.1	1.0	1.5	0.9	1.3	1.194
12	0.2	0.5	0.8	0.1	0.3	0.2	1.1	0.9	1.1	0.3	1.2	0.4	0.6	0.4	0.7	0.1	0.5	0.4	1.054
13	1.2	1.3	1.8	1.2	1.5	1.1	1.2	1.2	1.5	0.9	2.6	1.1	1.1	1.3	1.1	1.3	1.0	1.3	1.056
14	1.6	1.8	1.0	1.0	0.8	1.2	1.1	1.4	1.4	1.5	2.2	1.1	1.1	0.3	1.1	1.5	0.8	1.1	0.137
15	1.4	1.2	1.3	1.3	1.3	1.4	1.1	1.5	1.6	1.2	2.5	1.1	1.4	0.9	1.1	1.2	0.9	1.3	0.333
16	1.6	1.2	1.3	1.2	1.2	1.3	1.2	1.5	1.8	1.3	2.3	1.1	1.8	0.5	1.1	1.5	0.8	1.3	1.684
17	1.2	1.1	1.6	1.2	1.1	1.1	1.2	1.3	1.6	0.9	1.6	1.0	1.0	1.2	1.1	1.4	0.9	1.2	0.112
18	0.8	1.7	1.8	0.8	0.9	1.0	1.0	1.0	1.3	1.4	1.3	0.8	1.0	1.0	0.9	0.8	0.8	1.0	0.897
19	2.2	1.3	1.6	1.5	1.2	1.7	1.1	1.5	1.4	1.2	1.2	1.2	1.2	1.0	1.1	1.5	0.8	1.3	0.534
20	1.1	1.8	2.0	1.0	1.0	1.0	1.0	1.8	1.2	1.3	2.3	1.0	1.3	1.3	1.1	1.0	1.0	1.2	0.343
21	1.3	1.6	1.2	0.9	3.7	1.1	1.3	1.6	1.7	1.6	1.7	1.0	1.4	0.8	1.1	1.4	0.9	1.3	0.536
22	1.5	1.7	1.9	1.6	1.3	1.4	1.2	1.5	1.1	1.0	1.3	1.2	1.1	2.0	1.2	1.5	1.1	1.4	0.880
23	1.2	1.1	1.0	1.6	1.0	1.2	1.1	1.3	1.4	0.9	2.3	0.8	1.2	0.9	1.0	1.1	0.8	1.1	1.648