applied sciences

MDPI

Human Health Risk Associated with As, Cu, Pb, and Zn in Soils of the Aconcagua and Casablanca River Basins, Valparaíso Region, Chile

Jaume Bech[1], Daniela Pradenas[2], Pedro Tume[2,3*], Óscar Cornejo[2], Javiera Pedreros[2], Sofía Toledo[2], Claudio Correa[2], Bernardo Sepúlveda[4] and Núria Roca[1]

[1] Department Biologia Evolutiva, Ecologia i Ciències ambientals, Facultat de Biologia, Universitat de Barcelona, Av. Diagonal 643, 08023 Barcelona, Spain; jaumebechborras@gmail.com (J.B.); nroca@ub.edu (N.R.);
[2] Facultad de Ingeniería, Universidad Católica de la Santísima Concepción, Concepción 4090541, Chile; ptume@ucsc.cl (P.T.); dpradenas@ing.ucsc.cl (D.P.); ocornejo@ucsc.cl (O.C); jpedreros@ing.ucsc.cl (J.P.); sofiatoledo@ucsc.cl (S.T.); claudiocorrea@ucsc.cl (C.C)
[3] Centro de Investigación en Biodiversidad y Ambientes Sustentables (CIBAS), Universidad Católica de la Santísima Concepción, Concepción 4090541, Chile
[4] Centro Regional de Investigación y Desarrollo Sustentable de Atacama (CRIDESAT), Universidad de Atacama, Copiapó 1532297, Chile; bernardo.sepulveda@uda.cl
* Correspondence: ptume@ucsc.cl;

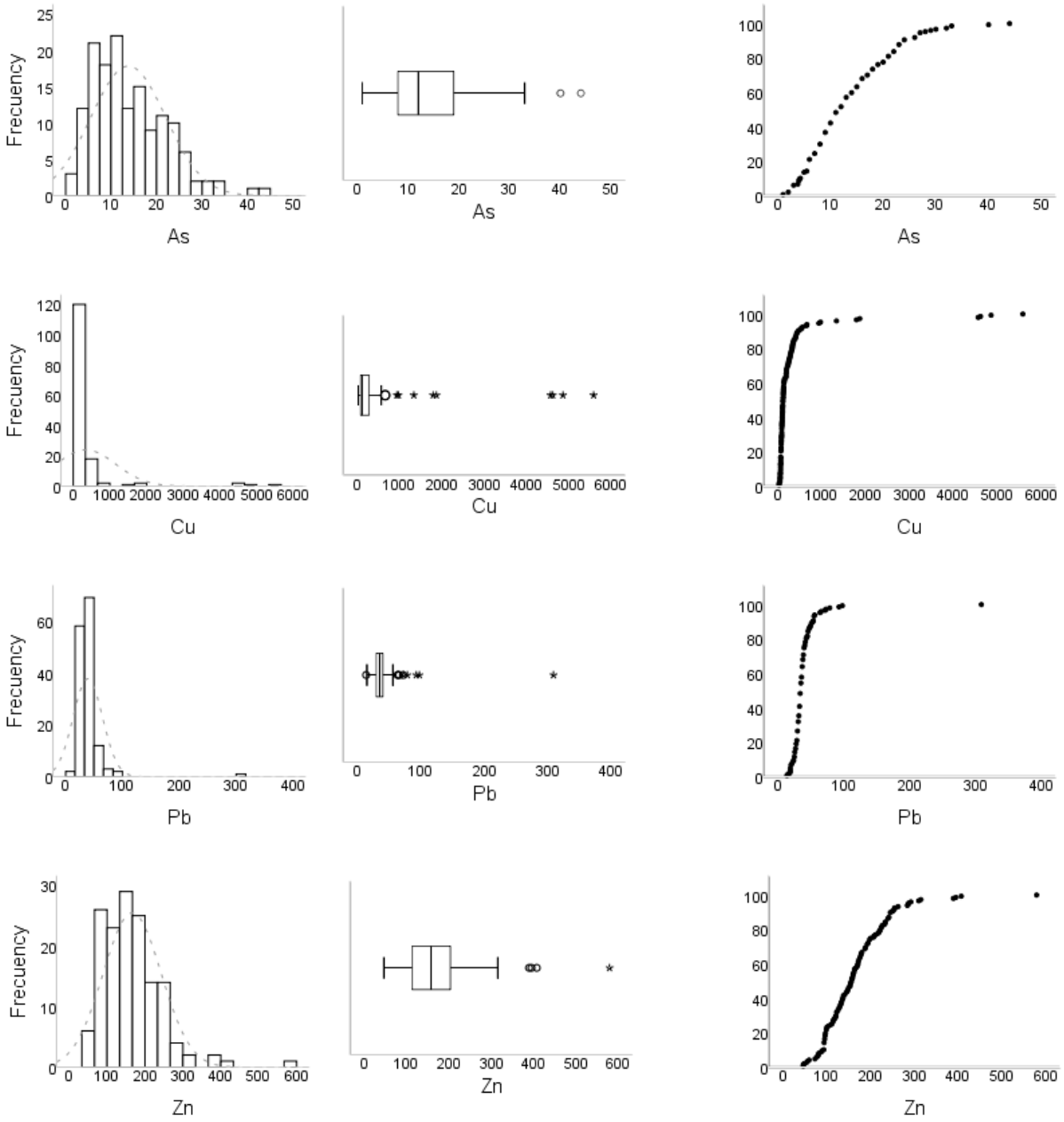

Figure S1: Graphical representation of the concentrations of heavy metals As, Cu, Pb and Zn (mg/kg) using histogram, box plot and CDF diagrams respectively for the soil of the Aconcagua River basin.

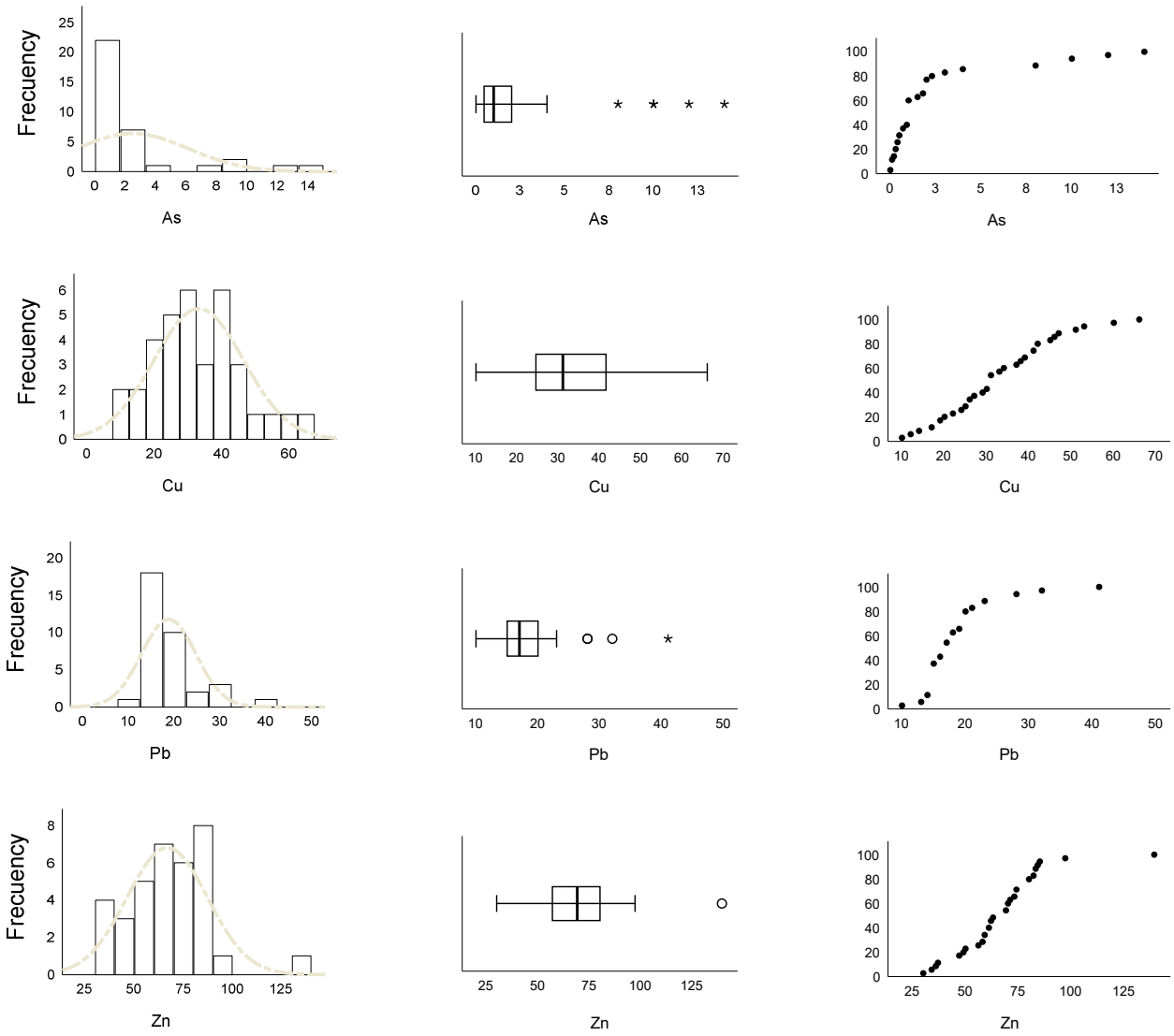

Figure S2: Graphical representation of the concentrations of heavy metals As, Cu, Pb and Zn (mg/kg) using histogram, box plot and CDF diagrams respectively for the soil of the Casablanca River basin.

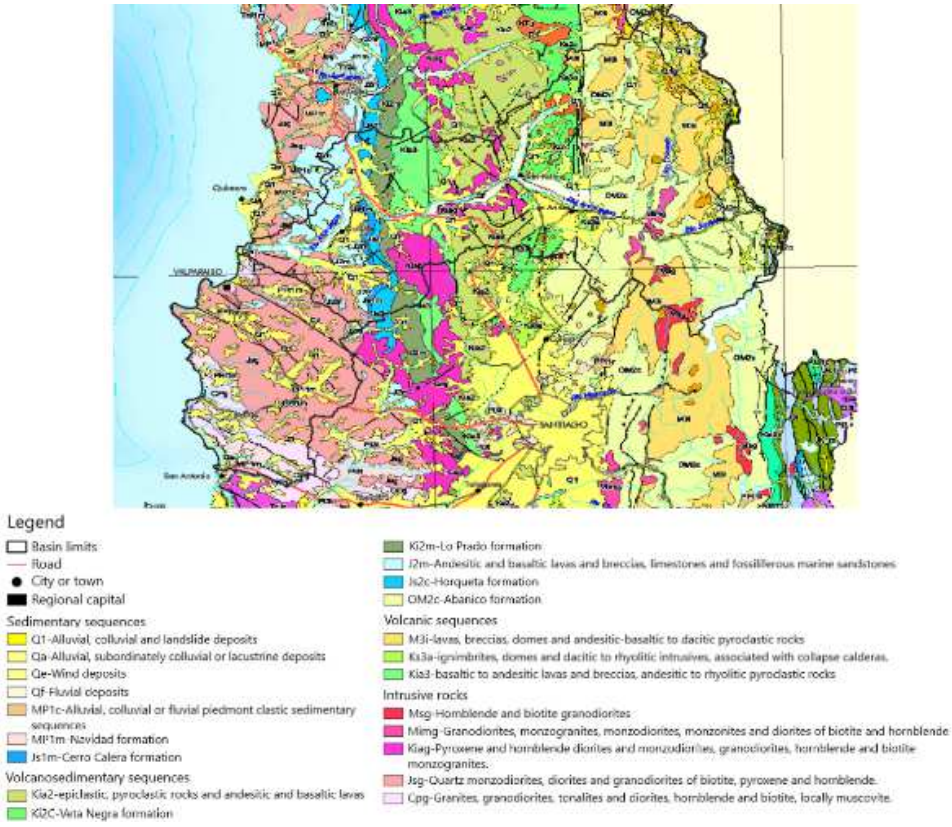

Figure S3. Geological map of the Aconcagua River basin

Equation S1. Positive matrix factorization

$$x_{ij} = \sum_{k=1}^{p} g_{ik} \times f_{kj} + e_{ij} \quad (1)$$

where:

The measured concentration of pollutants sample i. This is the observed data, typically the concentrations of various species (e.g., heavy metals) collected from environmental monitoring.

g_{ik} : the contribution of the source k to sample i, also known as the source contribution or source strength. This represents how much pollution from source k ends up in the sample i.

f_{kj} : the source profile for source k and pullant j, which is the characteristic concentration of pullant j emitted by the source k. This tells you the typical makeup of emissions from a particular source (e.g., how much As or Pb is typically emitted by a smelting facility).

e_{ij} : the residual or error term represents the part of the observed concentration that x_{ij} that is not explained by the modeled contributions of sources.

p : the total number of sources contributing to the measured concentrations.

Table S1: Classification of geoaccumulation

Igeo Value	Igeo Classification	Pollution level
<0	0	Not contaminated
0-1	1	Uncontaminated to moderately contaminated
1-2	2	Moderately contaminated
2-3	3	Moderately to heavily polluted
3-4	4	Heavily contaminated
4-5	5	From heavily polluted to extremely polluted
>5	6	extremely polluted

Table S2: Classification of soil contamination factor

CF Rating	Pollution Level
CF < 1	Low pollution
1 ≤ CF < 3	Moderate pollution
3 ≤ CF < 6	Considerable Pollution
CF ≥ 6	Very high pollution

Table S3. Variogram parameters for kriging modeling

Potential toxic element	As	Cu	Pb	Zn
Variogram model	spherical	exponential	exponential	spherical
Sill	0.06	0.09	0.05	0.07
Range	2235	8413	7200	3200
Nugget	0.02	0.06	0.02	0.03

Equation S2. Human intake through ingestion (DEing), dermal absorption (DEder), and inhalation (DEinh)

Exposure through soil and dust ingestion

$$DE_{ING} = \frac{Cs \times IngR \times EF \times ED \times Cf}{AT \times BW}$$

with

DE_{ING} = Dose of exposure through ingestion ($mg/(kg \times day)$)

Cs = Total contaminant concentration in soil (mg/kg)

$IngR$ = Ingestion rate (mg/day)

EF = Exposure frequency (days/year)

ED = Exposure duration (year)

CF = Conversion factor $1x10^{-6}$ (kg/mg)

BW = Body weight (kg)

AT = Averaging time during exposure (day)

Inhalation exposure

$$DE_{INH} = \frac{Cs \times InhR \times EF \times ED}{PEF \times BW \times AT}$$

where

DE_{INH} = Dose of exposure through ingestion ($mg/(kg \times day)$)

Cs = Total contaminant concentration in soil (mg/kg)

$InhR$ = Inhalation rate (m^3/days)

EF = Exposure frequency (days/year)

ED = Exposure duration (año)

PEF = Particle emission factor (m^3/kg)

BW = Body weight (kg)

AT = Averaging time during exposure (days)

Dermal contact exposure

$$DE_{DER} = \frac{Cs \times SA \times SAF \times ABSd \times EF \times ED \times CF}{BW \times AT}$$

where,

DE_{DER} = Dermal exposure dose ($mg/(kg \times day)$)

Cs = Contaminant concentration in soil (mg/kg)

SA = Skin surface area available for contact (cm^2/day)

SAF = Dermal adherence factor (mg/cm^2)

$ABSd$ = Dermal absorption factor (dimensionless)

EF = Exposure frequency (days/year))

ED = Exposure duration (years)

CF = Conversion factor $1x10^{-6}$(kg/mg)

BW = Body weight (kg)

AT = Averaging time for daily dose (days)

Table 5 shows the factors and values used in this study to calculate DE_{ING}, DE_{INH} and DE_{DER} for adults and children.

Equation S3. The noncarcinogenic risk for each element in the sample can be obtained as follows according to [32]:

$$HQ = HQing + HQinh + HQder$$

with

$$HQing = \frac{DEing}{RfDo}; HQinh = \frac{DEinh}{RfDinh}; HQder = \frac{DEder}{RfDder}$$

Equation S4: Cancer risk (CR_{SI}) is given by the following equation, which also considers the three exposure pathways as follows according to [32]:

$$CR_{SI} = CR_{ing} + CR_{der} + CR_{inh}$$

where $CR_{ing} = DEing \times SFo$; $CR_{der} = DEder \times SFd$; $CR_{inh} = DEinh \times SFi$ $DEing, DEder, DEinh$ are previously determined and SFo are the oral slope factor $(mg/kg \times days)^{-1}$, SFd : dermal slope factor $(mg/kg \times days)^{-1}$, and SFi : inhalation slope factor $(mg/kg \times days)^{-1}$.

Table S3. Values of the factors used in the equations referred to intake.

		Exposure Scenario		
	Factor (unit)	Adults	Children	Reference
Ingestion rate	IngR (mg/day)	100	200	[32]; [39]
Exposure frequency	EF (day/year)	350	350	[32]; [39]
Particulate emission factor	PEF (m^3/kg)	$1{,}36x10^9$		[32]; [39]
Exposure duration	ED (year)	30	6	[32]; [39]
Average exposure time (no carcinogenic)	AT (day)	Ed x 365		[32]; [39]
Average exposure time (carcinogenic)	AT (day)	70 x 365		[32]; [39]
body weight	BW (kg)	70	15	[32]; [39]
Skin adhesion factor	SAF (mg/cm^2)	0,07	0,2	[32]; [39]
Surface area	SA (cm^2/day)	5700	2800	[32]; [39]
Inhalation rate	InhR (m^3/day)	20	7,6	[32]; [37]; [39]
Dermal absorption factor	ABS_d (As)	0,03		[32]; [39]
	ABS_d (Cu, Pb y Zn)	0,001		[32]; [39]

Table S4. Factors used to calculate carcinogenic and no carcinogenic risk

		As	Cu	Pb	Zn	Reference
Oral reference dose	RfDo (mg/kgday)	0,0003	0,04	0,0035	0,3	[32]; [33]; [40]; [41]; [42]
Dermal reference dose	RfDder (mg/kgday)	0,000123	0,012	0,000525	0,06	[32]; [33]; [40]; [41]; [42]
Inhalation reference dose	RfDinh (mg/kgday)	0,0000086	0,04	0,0035	0,3	[32]; [33]; [40]; [41]; [42]
Oral slope factor	SF_o $(mg/kgday)^{-1}$	1,5	-	$8{,}5x10^{-4}$	-	[42]
Inhalation slope factor	SF_i $(mg/kgday)^{-1}$	15	-	0,28	-	[42]
Dermal slope factor	SF_d $(mg/kgday)^{-1}$	3,7	-	$8{,}5x10^{-4}$	-	[42]