

Article

Geochemical Signature and Risk Assessment of Potential Toxic Elements in Intensively Cultivated Soils of Southwestern Punjab, India

Supplementary Figures:

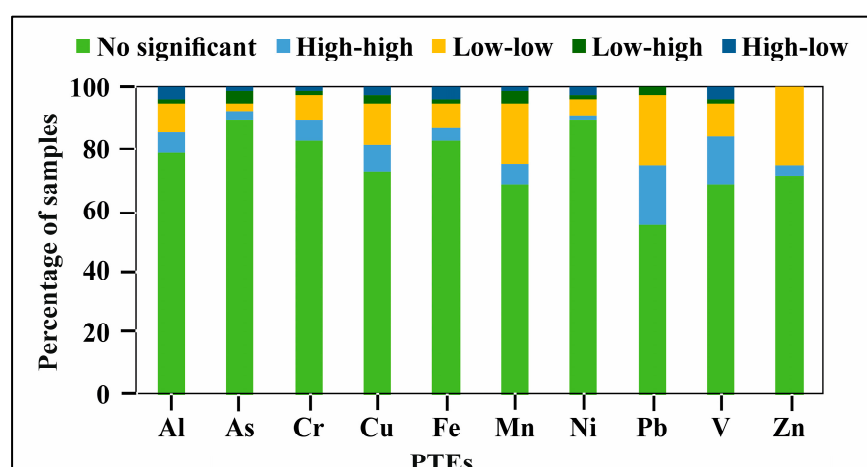


Figure S1. Distribution of different cluster groups of different PTEs. Indicates that most of the samples for all PTEs were in the no significant category.

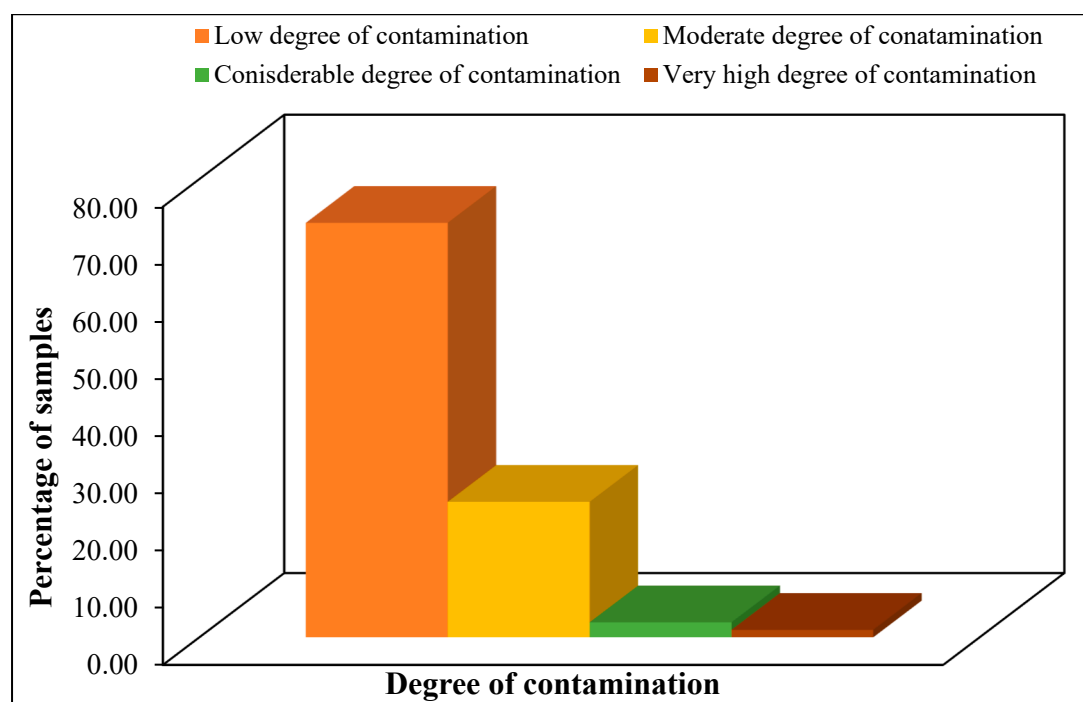


Figure S2. % of samples that belong to different levels of C_{deg} . Indicates that most of the samples exhibited a low degree of contamination or a moderate degree of contamination, whereas a very-low percentage of samples were in the considerable and very-high degree of contamination categories.

Supplementary Tables:

Table S1. Classification according to contamination factor [69].

Class	Contamination Factor (CF)
$CF < 1$	Low
$1 \leq CF < 3$	Moderate
$3 \leq CF < 6$	Considerable
$CF \geq 6$	Very high

Table S2. Classification according to degree of contamination [70].

Class	Degree of contamination level (Cdeg)
$C_{deg} < 8$	Low degree of contamination
$8 \leq C_{deg} < 16$	Moderate degree of contamination
$16 \leq C_{deg} < 32$	Considerable degree of contamination
$C_{deg} > 32$	Very high degree of contamination

Table S3. Classification according to Igeo values [71].

Class	Value	Soil Quality
0	$I_{geo} \leq 0$	Uncontaminated
1	$0 < I_{geo} < 1$	Uncontaminated/moderately contaminated
2	$1 < I_{geo} < 2$	Moderately contaminated
3	$2 < I_{geo} < 3$	Moderately/strongly contaminated
4	$3 < I_{geo} < 4$	Strongly contaminated
5	$4 < I_{geo} < 5$	Strongly/extremely contaminated
6	$5 < I_{geo}$	Extremely contaminated

Table S4. Moran's index, p-value, and z-score of different PTEs in soil, showed Pb has a MI value maximum of 0.53 with a p-value <0.001 that depicts the +ve spatial autocorrelation of Pb.

Parameters	Moran's Index	p-value	Z-value
Aluminum (Al)	0.186	0.01	2.7027
Arsenic (As)	-0.026	0.434	-0.2077
Chromium (Cr)	0.221	0.002	3.219
Copper (Cu)	0.207	0.002	3.1568
Iron (Fe)	0.041	0.222	0.7679
Manganese (Mn)	0.219	0.007	3.2527
Nickel (Ni)	0.043	0.207	0.8328
Lead (Pb)	0.530	0.001	7.4152
Vanadium (V)	0.363	0.001	5.2182
Zinc (Zn)	0.074	0.064	1.8639

Table S5. CF of selected PTEs in soil of semiarid region of Punjab.

PTEs	Min	Max	Average
Zn	0.015292	14.32802	0.995108
Cu	0.100766	1.485461	0.426633
Pb	0.007099	6.303831	1.112293
Mn	0.000186	1.176988	0.326336
V	0.130625	9.819063	4.029751
Ni	0.044944	0.955056	0.222717
Al	0.006926	0.669248	0.230835

Cr	0.089298	0.693371	0.324191
As	0.061404	0.22807	0.150161
Fe	0.0422	3.343688	1.038235

Table S6. The % of samples that belong to different classes on the basis of Igeo values of different PTEs in the soil. Indicates that most of the samples were in the uncontaminated category and very few samples of Pb, Zn, and V were in the uncontaminated/moderately-contaminated-to-moderately-contaminated category.

Class (%)	Classification	Zn	Cu	Pb	Mn	V	Ni	Al	Cr	As	Fe
0	Uncontaminated	92.1	100.0	75.0	100.0	13.2	100.0	100.0	100.0	100.0	85.5
1	Uncontaminated/moderately contaminated	5.3	0	10.5	0	28.9	0	0	0	0	13.2
2	Moderately contaminated	0	0	13.2	0	40.8	0	0	0	0	1.3
3	Moderately/strongly contaminated	1.3	0	1.3	0	17.1	0	0	0	0	0
4	Strongly contaminated	1.3	0	0	0	0	0	0	0	0	0
5	Strongly/extremely contaminated	0	0	0	0	0	0	0	0	0	0
6	Extremely contaminated	0	0	0	0	0	0	0	0	0	0

Table S7. Hazard quotient and hazard index of PTEs in children and adults.

	Min	Max	Average	Median
Children				
Zn	0.000251	0.235053	0.016387	0.01168
Cu	0.001377	0.020293	0.005857	0.005108
Pb	0.001391	1.235398	0.220072	0.079833
Ni	6.99E-10	1.49E-08	3.44E-09	3.38E-09
HI	0.009293	1.249231	0.242316	0.112115
Adult				
Zn	3.6E-05	0.033711	0.00235	0.001675
Cu	0.000198	0.002912	0.00084	0.000733
Pb	0.000199	0.177042	0.031538	0.011441
Ni	4.2E-10	8.94E-09	2.07E-09	2.03E-09
HI	0.001333	0.179027	0.034729	0.016071

Table S8. Cancer risk from As, Ni, and Cr in children and adults. Indicates all the samples belong to no-risk category.

	Min	Max	Average	Median
Children				
As	1.01E-05	3.77E-05	2.48E-05	2.46E-05
Ni	1.76E-08	3.74E-07	8.73E-08	8.52E-08
Cr	2.89E-06	1.07E-05	7.07E-06	7.02E-06
Adult				
As	1.45E-06	5.4E-06	3.56E-06	3.53E-06
Ni	1.06E-08	2.25E-07	5.25E-08	5.13E-08
Cr	4.19E-08	3.26E-07	1.52E-07	1.49E-07

Table S9. Summary of reference dose (RfD) and cancer slope factor (SF) of heavy metals through oral, dermal, and inhalation pathways [3,73,76].

Metals	Oral RfD	Dermal RfD	Inhalation RfD	Oral SF	Dermal SF	Inhalation SF
	(mg kg ⁻¹ day ⁻¹)	(mg kg ⁻¹ day ⁻¹)	(mg kg ⁻¹ day ⁻¹)	(mg kg ⁻¹ day ⁻¹)	(mg kg ⁻¹ day ⁻¹)	(mg kg ⁻¹ day ⁻¹)
Pb	1.40 E-03	5.24 E-04	5.71 E-05	NA	NA	NA
Cr	NA	NA	NA	NA	NA	4.20 E+01
Cu	2.00 E-02	5.40 E-03	NA	1.70 E+00	4.25 E+01	NA
Zn	4.00 E-02	1.20 E-02	NA	NA	NA	NA
Ni	NA	NA	3.00 E-01	NA	NA	8.40 E+01
As	NA	NA	NA	1.50 E+00	3.66 E+00	1.51 E+01

Table S10. Outcome of PCA. Indicated PC1 was positively loaded with Zn, Mn, V, and Al. PC2 was positively loaded with Pb, Mn, and Cu. PC3 was loaded with HCO₃⁻ and Mn.

	PC1	PC2	PC3	PC4	PC5
pH	0.0026181959	0.005552732	0.002095282	-0.0174971548	-0.024602262
EC	0.0142814017	0.131990642	-0.315152518	0.4741016300	-0.030203469
Salinity	0.0104648865	0.133884945	-0.320012308	0.4840771730	-0.025241182
HCO ₃ ⁻	0.2129572743	-0.140434307	0.041396170	-0.1194296205	-0.090970079
TKN	0.1220601482	-0.056162763	-0.064425435	0.2277909015	-0.017233114
AP	0.0271159394	-0.024652738	-0.001599773	0.0566769502	-0.053479917
TOC	0.2204656560	-0.088754616	-0.100186780	0.3163215021	0.088312844
Zn	0.5226350931	-0.038928018	0.293659186	0.0102652186	0.005573638
Cu	0.2019299501	0.206022836	-0.278350744	0.0002913704	-0.133298300
Pb	-0.2437739434	0.803979240	0.228845897	0.0752229254	-0.003391997
Mn	0.4058843714	0.288717359	0.526526151	0.1726163611	0.130164058
V	0.3423293564	0.075667652	-0.261354055	-0.1129788252	-0.080415125
Ni	-0.0903132173	0.091677429	-0.190109969	-0.1823711889	0.880269012
Al	0.3167705339	0.199621069	-0.240937183	-0.2994617966	-0.003303144
Cr	0.1522922792	0.164694401	-0.243128557	-0.0183640325	0.024975175
As	-0.0004117321	0.018182058	-0.060910239	0.0217197109	-0.004947832
Fe	0.2661820926	0.169783869	-0.226936556	-0.3050639451	0.025202152