Electronic Supplementary Material (ESI) for Environmental Science: Advances.

Layer-wise physicochemical and elemental distribution in an urban river water, Bangladesh: potential pollution, sources, and human health risk assessment

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Table S1. The limit of quantification (LOQ), the limit of detection (LOD), calibration range, and measurement uncertainty for the analyzed elements and anions.

Parameters	LOQ (µg/L)	LOD (µg/L)	Calibration range (µg/L)	Measurement uncertainty (±) (K=2)
As	2	0.2	2-20	16%
Cd	1	0.3	1-3	16.8%
Pb	5	1.2	5-15	31%
Hg	1	0.3	1-20	6.2%
Cr	5	0.4	5-15	20.8%
Ni	25	2.2	25-75	23.4%
Cu	100	6.2	100-2000	7.2%
Fe	100	67.7	100-2000	8%
Mn	50	3.1	50-1000	7%
Zn	50	7.5	50-1000	11.6%
F^-	500	30	500-2000	7.8%
Cl^-	500	90	500-2000	17.1%
SO_4^{2-}	1000	100	1000-4000	19.4%

Table S2. Description of the contamination indices and ecological risk assessment indices used in this study.

Index and formula	Descriptions	Standards	References
Heavy metal evaluation index (HEI): $HEI = \sum_{i=1}^{n} \frac{M_i}{S_i}$	HEI, broadly used for assessment of overall quality of the water with respect to toxic metals. Where, M_i and S_i represent the measured value and maximum admissible concentration (MAC) of the ith parameter, respectively.	HEI <10 (Low Risk), HEI = 10-20 (Medium Risk), and HEI > 20 (High Risk)	Edet and Offiong (2002) Mokarram et al. (2020) Siddique et al. (2021) Proshad et al. (2021)
Contamination degree (CD): $CF_i = [\frac{(CA_i)}{(CN_i)} - 1]$ $CD = \sum_{i=1}^{n} CF_i$	CD showed the collective effects of the water-quality parameters which are considered harmful to domestic water usage. Where, CFi, CAi, and CNi are the contamination factor, measured concentrations, and upper permissible concentration of ith parameter, respectively. 'N' indicates the 'normative value' while CNi is considered as MAC.	CD <4: Low Risk CD =4-8 : Medium Risk CD >8 : High Risk	Edet and Offiong (2002) Kabir et al. (2020) Siddique et al. (2021)
Potential ecological risk (PER): $C_f^i = C_m^i / C_n^i$ $E_r^i = C_f^i \times T_f^i$ $PER = \sum_{i=1}^{n} E_r^i$	E_r^i, Indicates sensitivity of the biotic community to the toxic elements and exemplifies the PER caused by the overall contamination. E_r^i is the potential ecological risk coefficient of a single metal; C_f^i is the accumulating coefficient of metal (i); T_f^i is the toxic-response factor of metal (i); C_m^i is the value of heavy metal concentration in the water samples; C_n^i is background values of corresponding metals (As=50, Cd=5, Pb=50, Cr=50, Ni=100, Cu=1000, Mn=100 and Zn=5000 μgL^{-1}); toxic-response factors for As, Cd, Pb, Cr, Ni, Cu, Mn and Zn were considered 10, 30, 5, 2, 5, 5, 1 and 1, respectively.	PER < 150: low, 150 < PER < 300: moderate, 300 < PER <600: considerable and 600 < PER: very high ecological risk.	ECR (1997) Proshad et al. (2021) Ukah et al. 2019 Egbueri (2020a) Egbueri (2020b)

Table S3. Definitions, symbols, units and values associated with equations used for health risk assessment.

Definitions	**Symbols**	**Units**	**Values**	**References**
Metal concentration	Cw	μg/L		
Body weight-adult	BWa	kg	70	Site-specific
Body weight-child	BWc	kg	15	USEPA (1991)
Resident/recreator exposure duration	ED	years	26	USEPA (2011)
Resident/recreator exposure duration-child	EDc	years	6	USEPA (1991)
Resident/recreator exposure duration-adult	EDa	years	20	USEPA (2020b)
Resident exposure frequency	EFres	days/year	350	USEPA (1991)
Recreator exposure frequency	EFrec	days/year	150	Site-specific
Resident exposure time-adult	ETres-a	hours/event	0.71	USEPA (2011)
Resident exposure time-child	ETres-c	hours/event	0.54	USEPA (2011)
Recreator exposure time-adult	ETrec-a	hours/event	2	Site-specific
Recreator exposure time-child	ETrec-c	hours/event	2	Site-specific
Resident/recreator events-adult	EVa	per day	1	USEPA (2004)
Resident/recreator events-child	EVc	per day	1	USEPA (2004)
Resident/recreator skin surface area-adult	SAa	cm^2	19652	USEPA (2014)
Resident/recreator skin surface area-child	SAc	cm^2	6365	USEPA (2014)
Resident water intake ratio-adult	IRWres-a	L/day	2.5	USEPA (2011)
Resident water intake ratio-child	IRWres-c	L/day	0.78	USEPA (2011)
Recreator water intake ratio-adult	IRWrec-a	L/day	0.11	USEPA (2011)
Recreator water intake ratio-child	IRWrec-c	L/day	0.12	USEPA (2011)
Resident averaging time-adult	ATres-a	days	365 x ED = 9490 (non-carcinogenic)	USEPA (1989)
Resident averaging time-child	ATres-c	days	365 x EDc = 2190 (non-carcinogenic)	USEPA (1989)
Recreator averaging time-adult	ATrec-a	days	365 x Eda = 7300 (non-carcinogenic)	USEPA (1989)
Recreator averaging time-child	ATrec-c	days	365 x Edc =2190 (non-carcinogenic)	USEPA (1989)
Resident water ıngestion rate	IFWres	L/kg	Age-adjusted	USEPA (2020b)
Recreator water ıngestion rate	IFWrec	L/kg	Age-adjusted	USEPA (2020b)
Resident water dermal contact factor	DFWres	cm^2 -event/kg	Age-adjusted	USEPA (2020b)

Recreator water dermal contact factor	DFWrec	cm^2 -event/kg	Age-adjusted	USEPA (2020b)
Resident water exposure time	ETevent-res	hours/event	Age-adjusted	USEPA (2020b)
Recreator water exposure time	ETevent-rec	hours/event	Age-adjusted	USEPA (2020b)
Life time	LT	years	70	USEPA (1989)
Averaging time	AT	days	365 × LT = 25550 (carcinogenic)	USEPA (1989)

Table S4. Dermal permeability coefficient, reference dose, slope factor and gastrointestinal absorption coefficient for each element.

Element	Dermal permeability constant (Kp; cm/h)[a]	Oral reference dose (RfDo; mg/kg-day)[b]	Oral slope factor (CSFo; mg/kg-day)[b]	Gastrointestinal absorption (GIABS; unitless)[b]
As	0.001	0.0003	1.5	1
Cd	0.0001	0.001		1
Pb	0.0001	0.0014	0.0085	1
Hg	0.001	0.0002		1
Cr	0.002	0.003	0.5	0.025
Ni	0.0002	0.02		0.04
Cu	0.001	0.04		1
Fe	0.001	0.7		1
Mn	0.001	0.024		0.04
Zn	0.0006	0.3		1

[a]USEPA (2004) [b]USEPA (2020c)

Table S5. Pearson's Correlation analysis for heavy metals concentrations in the surface water of the Buriganga River for wet season.

Wet season	As	Cd	Pb	Hg	Cr	Ni	Cu	Fe	Mn	Zn
As	1.000									
Cd	0.575	1.000								
Pb	0.258	0.650	1.000							
Hg	0.382	0.642	0.850	1.000						
Cr	0.122	0.315	0.440	0.321	1.000					
Ni	0.124	0.461	0.681	0.681	0.311	1.000				
Cu	-0.310	0.383	0.498	0.375	0.205	0.424	1.000			
Fe	-0.037	0.358	0.378	0.311	0.197	-0.085	0.587	1.000		
Mn	-0.255	-0.099	0.011	0.016	0.248	-0.257	-0.116	0.080	1.000	
Zn	-0.185	0.236	0.773	0.539	0.186	0.390	0.627	0.446	0.035	1.000

Table S6. Pearson's Correlation analysis for heavy metals concentrations in the deep water of the Buriganga River for wet season.

Wet season	As	Cd	Pb	Hg	Cr	Ni	Cu	Fe	Mn	Zn
As	1.000									
Cd	0.591	1.000								
Pb	0.760	0.723	1.000							
Hg	0.879	0.733	0.921	1.000						
Cr	0.519	0.339	0.355	0.447	1.000					
Ni	0.643	0.705	0.733	0.773	0.564	1.000				
Cu	0.690	0.595	0.927	0.830	0.250	0.576	1.000			
Fe	0.869	0.580	0.799	0.814	0.511	0.539	0.752	1.000		
Mn	0.799	0.460	0.655	0.823	0.620	0.687	0.572	0.714	1.000	
Zn	0.591	0.704	0.737	0.719	0.360	0.504	0.733	0.634	0.514	1.000

Table S7. Pearson's Correlation analysis for heavy metals concentrations in the surface water of the Buriganga River for dry season.

Dry season	As	Cd	Pb	Hg	Cr	Ni	Cu	Fe	Mn	Zn
As	1.000									
Cd	0.655	1.000								
Pb	0.599	0.919	1.000							
Hg	0.627	0.797	0.769	1.000						
Cr	0.559	0.427	0.474	0.628	1.000					
Ni	0.513	0.491	0.648	0.620	0.676	1.000				
Cu	0.350	0.270	0.320	0.600	0.464	0.629	1.000			
Fe	0.571	0.816	0.753	0.886	0.316	0.530	0.476	1.000		
Mn	0.754	0.836	0.849	0.799	0.723	0.594	0.377	0.661	1.000	
Zn	0.315	0.694	0.697	0.458	-0.077	0.093	0.196	0.550	0.524	1.000

Table S8. Pearson's Correlation analysis for heavy metals concentrations in the deep water of the Buriganga River for dry season.

Dry season	As	Cd	Pb	Hg	Cr	Ni	Cu	Fe	Mn	Zn
As	1.000									
Cd	0.735	1.000								
Pb	0.836	0.750	1.000							
Hg	0.896	0.773	0.839	1.000						
Cr	0.611	0.737	0.596	0.727	1.000					
Ni	0.729	0.714	0.832	0.814	0.667	1.000				
Cu	0.778	0.778	0.790	0.778	0.732	0.705	1.000			
Fe	0.778	0.450	0.594	0.616	0.278	0.548	0.641	1.000		
Mn	0.637	0.529	0.691	0.660	0.747	0.741	0.741	0.461	1.000	
Zn	0.830	0.589	0.602	0.723	0.312	0.428	0.627	0.783	0.399	1.000

Table S9. Heavy metal evaluation index (HEI) and Degree of contamination (CD) of heavy metals in surface and deep water of the Buriganga River.

Sites	Heavy metal evaluation index				Degree of contamination			
	Surface water		Deep water		Surface water		Deep water	
	Dry season	Wet season	Dry season	Wet season	Dry season	Wet season	Dry season	Wet season
B1	51.7	40.1	40.5	27.6	99.0	68.5	76.8	46.1
B2	54.5	31.8	38.0	28.3	106.9	49.0	75.2	41.3
B3	51.9	28.7	43.0	31.0	95.4	47.5	81.3	46.9
B4	44.9	27.1	45.9	33.9	75.6	49.5	84.5	51.4
B5	55.0	38.8	50.8	31.6	95.7	57.7	88.5	54.5
B6	46.0	35.6	46.1	36.4	87.1	63.1	86.8	70.2
B7	44.1	35.4	42.8	36.2	73.6	65.2	87.9	68.6
B8	51.6	33.0	53.3	28.5	89.1	59.1	106.2	49.7
B9	59.3	35.4	49.1	36.0	115.9	70.7	101.0	69.3
B10	59.5	37.8	58.0	43.2	116.4	76.2	109.4	76.2
B11	65.0	39.0	59.5	45.1	125.6	84.6	124.8	90.6
B12	64.7	45.4	61.5	43.1	131.0	93.4	123.8	94.6
B13	69.0	54.1	63.5	47.7	143.8	100.3	138.3	106.8
B14	65.6	50.4	67.0	50.8	136.3	96.9	149.6	116.4
Average	55.9	38.0	51.4	37.1	106.5	70.1	102.4	70.2
SD	8.15	7.65	9.24	7.64	22.26	17.87	23.77	24.03

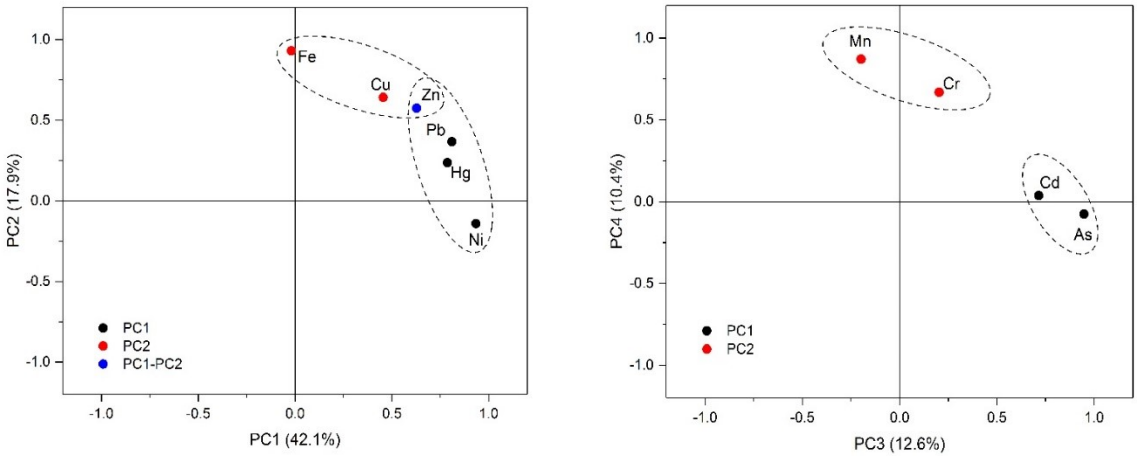
Table 10. Ecological risks of metals in the surface water of Buriganga river during dry and wet season.

Sites	As	Cd	Pb	Cr	Ni	Cu	Mn	Zn	PER	As	Cd	Pb	Cr	Ni	Cu	Mn	Zn	PER
Seasons					Dry									Wet				
B1	14.0	429	9.11	7.08	6.5	0.78	1.69	0.052	468.2	11.1	343.8	6	4.88	4.75	0.57	1.52	0.041	372.6
B2	15.6	453	9.94	6.24	7.1	0.77	1.67	0.058	494.3	6.16	270.6	3.95	5.28	5.35	0.73	1.56	0.035	293.7
B3	13.4	463.2	8.35	5.96	7.3	0.76	1.46	0.049	500.5	8.98	199.8	4.18	4.64	5.85	0.67	1.39	0.042	225.6
B4	11.0	390.6	6.17	6.96	6.65	0.89	1.53	0.048	423.9	8.22	153.6	4.78	5.04	6	0.68	1.48	0.041	179.8
B5	17.3	472.8	7.92	7.4	6.75	0.95	1.67	0.052	514.9	12.7	330.6	4.41	5.68	4.15	0.63	1.52	0.032	359.7
B6	10.4	391.8	7.9	5.92	7.4	1.03	1.42	0.055	425.9	8.80	289.8	5.67	4.68	6.1	0.78	1.32	0.041	317.2
B7	16.4	331.2	5.78	6.76	8.05	1.04	1.5	0.047	370.8	9.42	264	5.96	5.88	6.95	0.67	1.35	0.042	294.3
B8	15.8	451.2	7.48	5.76	5.7	0.84	1.57	0.054	488.4	8.88	246	5.69	5	4.1	0.73	1.36	0.052	271.8
B9	15.5	529.8	10.8	5.8	6.15	0.96	1.67	0.064	570.7	6.58	265.2	7.11	5.36	5.5	0.88	1.58	0.059	292.3
B10	15.6	510.6	10.6	6.72	8.2	0.94	1.75	0.058	554.5	6.72	293.4	7.59	5.64	6.15	0.79	1.52	0.052	321.9
B11	19.1	552.6	11.2	7.52	8.65	1.05	1.88	0.056	602.0	8.62	282.6	8.81	5.64	6.6	0.72	1.52	0.053	314.6
B12	17.7	543	12.2	7.68	8.6	0.98	1.79	0.058	592.0	12.0	359.4	9.13	5.4	7.25	0.68	1.49	0.052	395.4
B13	19.3	573.6	13.6	7.52	9.45	1.00	1.83	0.056	626.3	11.1	528	8.77	5.32	7.7	0.83	1.42	0.051	563.2
B14	16.4	550.8	12.9	7.68	9.15	1.07	1.9	0.056	599.9	11.2	459.6	8.9	5.64	7.2	0.89	1.37	0.050	494.8
Average	15.5	474.5	9.57	6.79	7.55	0.93	1.67	0.055	516.6	9.32	306.17	6.50	5.29	5.98	0.73	1.46	0.046	335.5
SD	2.63	72.5	2.44	0.73	1.16	0.11	0.15	0.005	77.62	2.05	96.68	1.88	0.39	1.13	0.09	0.09	0.01	99.8

Table S11. Ecological risks of metals in the deep water of Buriganga River during dry and wet season.

Sites	As	Cd	Pb	Cr	Ni	Cu	Mn	Zn	PER	As	Cd	Pb	Cr	Ni	Cu	Mn	Zn	PER
Seasons					Dry									Wet				
B1	10.2	337.2	0.29	5.32	5.25	0.71	1.28	0.050	360.3	6.64	234	4.33	3.464	4.195	0.52	1.03	0.029	254.2
B2	8.4	282	0.30	6	6	0.75	1.59	0.047	305.1	5.98	249	3.33	4.44	4.35	0.56	1.21	0.033	268.9
B3	11.1	354	0.31	5.68	5.6	0.75	1.33	0.048	378.8	6.78	283.8	3.87	4.36	4.15	0.545	1.09	0.047	304.6
B4	10.7	392.4	0.30	7.04	6.15	0.86	1.51	0.048	419.0	8.1	307.2	3.94	5.04	5.8	0.59	1.26	0.039	332.0
B5	10.9	472.2	0.30	7.4	6.4	0.92	1.61	0.047	499.8	8.24	238.2	5.13	5.4	3.945	0.615	1.38	0.035	262.9
B6	11.0	390.6	0.32	5.28	6.2	0.90	1.4	0.055	415.8	9.56	280.2	6.84	4.8	5.75	0.69	1.23	0.033	309.1
B7	8.78	337.2	0.34	6.16	7.7	0.80	1.49	0.040	362.5	5.42	319.8	6.49	5.4	6.45	0.545	1.28	0.040	345.4
B8	13.1	444.6	0.40	7.00	7.35	0.83	1.52	0.054	474.9	7.78	193.2	4.6	5.08	5.85	0.58	1.39	0.032	218.5
B9	16.5	336.6	0.40	6.72	6.85	0.95	1.62	0.055	369.7	10.9	253.8	6.77	5.44	5.5	0.635	1.3	0.041	284.3
B10	16.2	505.8	0.39	6.92	7.85	0.87	1.51	0.056	539.6	13.1	353.4	6.61	5.8	6.4	0.58	1.46	0.039	387.4
B11	17.1	466.8	0.48	7.12	8.1	0.93	1.75	0.056	502.3	13.9	333	8.79	5.24	6.65	0.695	1.68	0.045	370.0
B12	18.5	504	0.46	7.48	7.7	1.06	1.65	0.060	540.9	12.7	298.8	9.9	5.4	6.05	0.875	1.52	0.052	335.3
B13	15.6	529.8	0.55	7.56	7.75	1.02	1.58	0.052	563.9	11.1	366	11.2	5.68	6.5	0.89	1.43	0.049	402.8
B14	17.9	539.4	0.60	7.00	8.45	1.04	1.76	0.058	576.2	12.9	379.8	12.3	6.24	6.9	0.94	1.44	0.051	420.5
Average	13.3	420.9	0.39	6.62	6.95	0.88	1.54	0.052	450.6	9.51	292.2	6.72	5.13	5.61	0.66	1.34	0.040	321.2
SD	3.54	84.09	0.10	0.79	1.02	0.11	0.14	0.005	88.3	2.91	54.9	2.85	0.69	1.03	0.14	0.17	0.007	60.2

Supplementary Figures



(a) (b)

Fig. S1. Loading plot of PCA for heavy metals concentration in the surface water for wet season a) PC1-PC2, b) PC3-PC4.

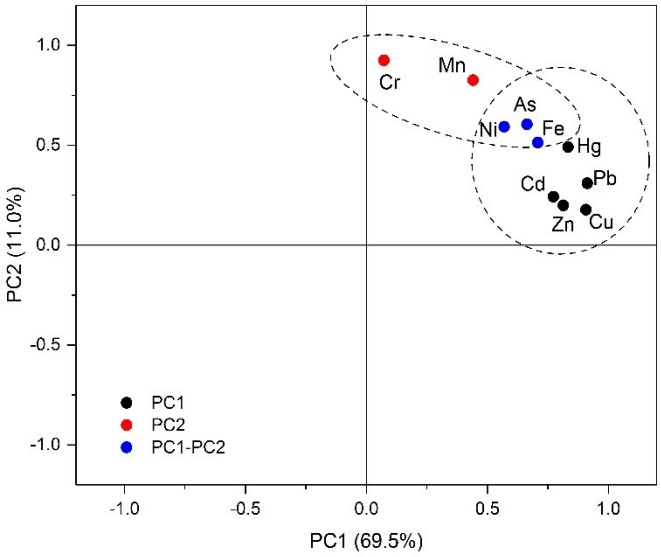


Fig. S2. Loading plot of PCA for heavy metals concentration in the deep water for wet season.

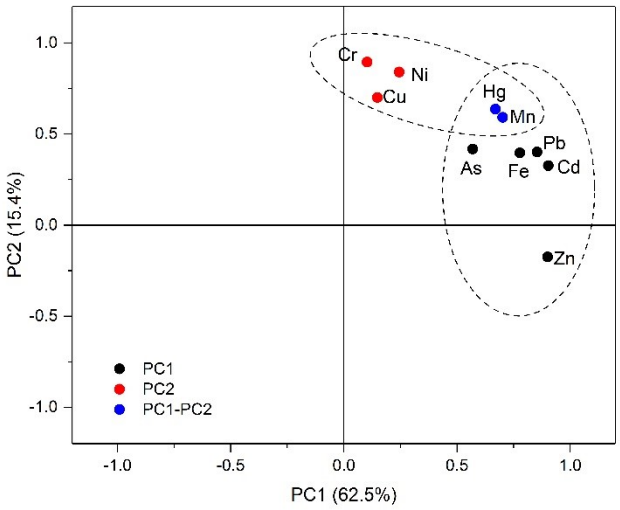


Fig. S3. Loading plot of PCA for heavy metals concentration in the surface water for dry season.

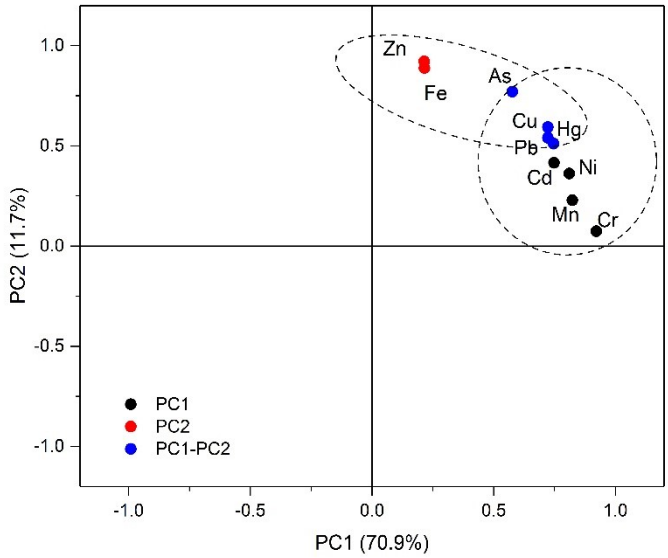


Fig. S4. Loading plot of PCA for heavy metals concentration in the deep water for dry season.

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