Supplementary Material

A comprehensive approach to the chemistry, pollution impact and risk assessment of drinking water sources in a former industrialized area of Romania

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Table S1. The metal detection limits (LOD) for the water samples analyzed by spectrometry methods

Element	Unit	LOD	Instrument
Ca	mg/L	0.004	ICP-OES
Mg	mg/L	0.009	ICP-OES
Na	mg/L	0.008	ICP-OES
K	mg/L	0.003	ICP-OES
Fe	mg/L	0.008	ICP-OES
Zn	µg/L	0.31	ICP-MS
Pb	µg/L	0.11	ICP-MS
Mn	µg/L	0.13	ICP-MS
Cu	µg/L	0.21	ICP-MS
Cd	µg/L	0.07	ICP-MS
Cr	µg/L	0.22	ICP-MS
Ni	µg/L	0.13	ICP-MS
As	µg/L	0.27	ICP-MS

Table S2. The limits of detection (LOD) for the anion determinations using liquid ion chromatography analysis by ion chromatograph and NH_4^+ using UV-VIS spectrometer

Element	Unit	LOD	Instrument
NO_2^-	mg/L	0.010	IC
NO_3^-	mg/L	0.100	IC
SO_4^{2-}	mg/L	0.011	IC
Cl^-	mg/L	0.004	IC
NH_4^+	mg/L	0.026	UV-VIS spectrometer

Table S3. The metallic impurities in the Multielement Calibration Standard 3, from Perkin-Elmer (Waltham, MA, USA)

Element	µg/L
Au	<0.06
B	4
Ce	0.04
Dy	0.03
Er	<0.01
Eu	<0.1
Gd	0.03
Ge	<0.5
Hf	<0.01
Hg	<0.3
Ho	<0.01
Ir	0.1
La	0.2
Lu	<0.01
Mo	0.7
Nb	<0.06
Nd	<0.02
P	<200
Pd	<3
Pr	<0.01

Pt	<0.02
Re	<0.01
Rh	<0.7
Ru	0.2
Sb	0.05
Sc	0.05
Si	<100
Sm	2
Sn	0.1
Ta	<0.03
Tb	<0.01
Te	<0.2
Th	<0.01
Ti	<8
Tm	0.05
W	<0.3
Y	0.2
Yb	<0.01
Zr	0.1

Table S4. The water samples Ca, Mg, K, and Fe contents

Sample	Ca mg/L	Mg mg/L	Na mg/L	K mg/L	Fe mg/L
1	115 ± 9.24	14.4 ± 1.15	37.8 ± 3.03	1.38 ± 0.11	0.050 ± 0.004
2	77.7 ± 6.21	12.0 ± 0.96	91.3 ± 7.30	13.6 v 1.09	0.044 ± 0.004
3	87.3± 6.98	16.4 ± 1.31	30.3 ± 2.42	2.78 ± 0.22	0.065 ± 0.005
4	113± 9.02	9.18 ± 0.73	53.9 ± 4.31	1.51± 0.12	0.044 ± 0.004
5	12.0± 0.96	21.3 ± 1.71	52.7 ± 4.22	9.13 ± 0.73	0.056 ± 0.004
6	65.0± 5.20	8.50 ± 0.68	8.54 ± 0.68	2.03 ± 0.16	0.030 ± 0.002
7	100± 8.02	10.0 ± 0.80	31.4 ± 2.52	8.07 ± 0.65	0.040 ± 0.003
8	130± 10.40	8.58 ± 0.69	28.6 ± 2.29	0.69 ± 0.06	0.040 ± 0.003
9	98.6± 7.88	19.3 ± 1.54	61.3 ± 4.90	16.6 ± 1.33	0.048 ± 0.004
10	69.9± 5.59	6.65 ± 0.53	28.6 ± 2.29	28.5 ± 2.28	0.039 ± 0.003
11	73.5 ± 5.88	13.7 ± 1.10	88.9 ± 7.11	25.0 ± 2.00	0.027 ± 0.002
12	75.9 ± 6.07	8.51 ± 0.68	31.4 ± 2.51	3.25 ± 0.26	0.048 ± 0.004
13	99.5 ± 7.96	13.1 ± 1.05	66.7 ± 5.34	6.93 ± 0.55	0.037 ± 0.003
14	128 ± 10.20	25.1 ± 2.01	61.5 ± 4.92	10.1 ± 0.81	0.066 ± 0.005
15	135 ± 10.80	8.21 ± 0.66	32.8 ± 2.63	1.01 ± 0.08	0.045 ± 0.004
min	**12.0**	**6.65**	**8.54**	**0.69**	**0.0269**
max	**135**	**25.1**	**91.3**	**28.5**	**0.0662**
average	**92.0**	**13.0**	**47.1**	**8.70**	**0.0453**

Table S5. The water samples Zn, Pb, Mn, Cu, Cd, Cr, Ni, and As contents

Sample	Zn µg/L	Pb µg/L	Mn µg/L	Cu µg/L	Cd µg/L	Cr µg/L	Ni µg/L	As µg/L
1	55.5 ± 4.44	0.51 ± 0.04	8.35 ± 0.67	3.73 ± 0.30	0.07 ± 0.01	3.71 ± 0.30	3.31 ± 0.27	0.54 ± 0.04
2	356 ± 28.5	0.27 ± 0.02	82.4 ± 6.59	9.00 ± 0.72	0.08 ± 0.01	4.34 ± 0.35	1.85 ± 0.15	<0.27
3	31.4 ± 2.51	<0.11	1.11 ± 0.09	6.83 ± 0.55	0.30 ± 0.02	11.2 ± 0.90	2.69 ± 0.22	<0.27
4	63.3 ± 5.07	0.27 ± 0.02	2.18 ± 0.17	5.16 ± 0.41	0.41 ± 0.03	3.63 ± 0.29	3.29 ± 0.26	0.90 ± 0.07
5	901 ± 72.1	12.0 ± 0.96	8.55 ± 0.68	8.09 ± 0.65	19.27 ± 1.54	5.93 ± 0.47	6.65 ± 0.53	6.70 ± 0.54
6	66.4 ± 5.31	0.29 ± 0.02	1.43 ± 0.11	2.66 ± 0.21	<0.07	3.16 ± 0.25	4.14 ± 0.33	<0.27
7	13.3 ± 1.06	0.26 ± 0.02	0.93 ± 0.07	3.93 ± 0.31	<0.07	3.67 ± 0.29	1.30 ± 0.10	<0.27
8	7.10 ± 0.57	0.81 ± 0.07	1.10 ± 0.09	0.58 ± 0.05	<0.07	3.48 ± 0.28	1.60 ± 0.13	<0.27
9	13.3 ± 1.06	0.28 ± 0.02	43.2 ± 3.45	5.00 ± 0.40	<0.07	5.48 ± 0.44	3.10 ± 0.25	<0.27
10	110 ± 8.77	0.53 ± 0.04	3.52 ± 0.28	8.17 ± 0.65	0.16 ± 0.01	1.89 ± 0.15	2.83 ± 0.23	2.27 ± 0.18
11	1910 ± 96	0.59 ± 0.05	65.9 ± 5.27	12.6 ± 1.01	<0.07	3.97 ± 0.32	1.49 ± 0.12	0.33 ± 0.03
12	57.3 ± 4.59	2.31 ± 0.18	1.04 ± 0.08	5.89 ± 0.47	<0.07	3.43 ± 0.27	1.70 ± 0.14	1.23 ± 0.10
13	35.0 ± 2.80	0.65 ± 0.05	0.31 ± 0.02	3.04 ± 0.24	<0.07	4.96 ± 0.40	1.61 ± 0.13	<0.27
14	22.4 ± 1.79	0.29 ± 0.02	10.0 ± 0.80	4.36 ± 0.35	<0.07	4.49 ± 0.36	3.48 ± 0.28	0.30 ± 0.02
15	102 ± 8.19	0.17 ± 0.01	1.10 ± 0.09	2.60 ± 0.21	<0.07	1.29 ± 0.10	1.64 ± 0.13	<0.27
min	***7.10***	***0.17***	***0.31***	***0.58***	***0.07***	***1.29***	***1.30***	***0.30***
max	***1910***	***12.01***	***82.4***	***12.6***	***19.3***	***11.2***	***6.65***	***6.70***
average	***250***	***1.28***	***15.41***	***5.44***	***3.38***	***4.31***	***2.71***	***1.75***

Table S6. The calculated Chronic Daily Intake (CDI) for all studied heavy metals, in the case of children

CDI	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Cu	3.73E-04	9.00E-04	6.83E-04	5.16E-04	8.09E-04	2.66E-04	3.93E-04	5.82E-05	5.00E-04	8.17E-04	1.26E-03	5.89E-04	3.04E-04	4.36E-04	2.60E-04
Fe	5.04E-03	4.45E-03	6.48E-03	4.40E-03	5.61E-03	3.04E-03	4.04E-03	4.03E-03	4.77E-03	3.87E-03	2.69E-03	4.83E-03	3.67E-03	6.62E-03	4.46E-03
Mn	8.35E-04	8.24E-03	1.11E-04	2.18E-04	8.55E-04	1.43E-04	9.27E-05	1.10E-04	4.32E-03	3.52E-04	6.59E-03	1.04E-04	3.11E-05	1.00E-03	1.10E-04
Zn	5.55E-03	3.56E-02	3.14E-03	6.33E-03	9.01E-02	6.64E-03	1.33E-03	7.10E-04	1.33E-03	1.10E-02	1.91E-01	5.73E-03	3.50E-03	2.24E-03	1.02E-02
Cr	3.71E-04	4.34E-04	1.12E-03	3.63E-04	5.93E-04	3.16E-04	3.67E-04	3.48E-04	5.48E-04	1.89E-04	3.97E-04	3.43E-04	4.96E-04	4.49E-04	1.29E-04
Ni	3.31E-04	1.85E-04	2.69E-04	3.29E-04	6.65E-04	4.14E-04	1.30E-04	1.60E-04	3.10E-04	2.83E-04	1.49E-04	1.70E-04	1.61E-04	3.48E-04	1.64E-04
Pb	5.08E-05	2.70E-05	0.00E+00	2.69E-05	1.20E-03	2.89E-05	2.60E-05	8.14E-05	2.79E-05	5.26E-05	5.86E-05	2.31E-04	6.48E-05	2.91E-05	1.73E-05
Cd	7.40E-06	7.90E-06	3.03E-05	4.12E-05	1.93E-03	4.10E-06	4.90E-06	6.40E-06	2.50E-06	1.63E-05	4.10E-06	4.10E-06	3.50E-06	8.00E-07	0.00E+00
min	7.40E-06	7.90E-06	0.00E+00	2.69E-05	5.93E-04	4.10E-06	4.90E-06	6.40E-06	2.50E-06	1.63E-05	4.10E-06	4.10E-06	3.50E-06	8.00E-07	0.00E+00
max	5.55E-03	3.56E-02	6.48E-03	6.33E-03	9.01E-02	6.64E-03	4.04E-03	4.03E-03	4.77E-03	1.10E-02	1.91E-01	5.73E-03	3.67E-03	6.62E-03	1.02E-02
average	1.57E-03	6.23E-03	1.48E-03	1.53E-03	1.27E-02	1.36E-03	7.98E-04	6.87E-04	1.48E-03	2.07E-03	2.53E-02	1.50E-03	1.03E-03	1.39E-03	1.92E-03

Table S7. The calculated Chronic Daily Intake (CDI) for all studied heavy metals, in the case of adults

CDI	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Cu	1.07E-04	2.57E-04	1.95E-04	1.47E-04	2.31E-04	7.59E-05	1.12E-04	1.66E-05	1.43E-04	2.33E-04	3.61E-04	1.68E-04	8.68E-05	1.24E-04	7.44E-05
Fe	1.44E-03	1.27E-03	1.85E-03	1.26E-03	1.60E-03	8.68E-04	1.16E-03	1.15E-03	1.36E-03	1.11E-03	7.68E-04	1.38E-03	1.05E-03	1.89E-03	1.27E-03
Mn	2.39E-04	2.36E-03	3.17E-05	6.22E-05	2.44E-04	4.08E-05	2.65E-05	3.13E-05	1.23E-03	1.00E-04	1.88E-03	2.96E-05	8.89E-06	2.86E-04	3.15E-05
Zn	1.58E-03	1.02E-02	8.96E-04	1.81E-03	2.58E-02	1.90E-03	3.79E-04	2.03E-04	3.79E-04	3.13E-03	5.46E-02	1.64E-03	9.99E-04	6.39E-04	2.93E-03
Cr	1.06E-04	1.24E-04	3.21E-04	1.04E-04	1.69E-04	9.02E-05	1.05E-04	9.95E-05	1.57E-04	5.41E-05	1.14E-04	9.79E-05	1.42E-04	1.28E-04	3.69E-05
Ni	9.47E-05	5.28E-05	7.69E-05	9.41E-05	1.90E-04	1.18E-04	3.73E-05	4.57E-05	8.86E-05	8.08E-05	4.24E-05	4.85E-05	4.59E-05	9.94E-05	4.67E-05
Pb	1.45E-05	7.71E-06	0.00E+00	7.69E-06	3.43E-04	8.26E-06	7.43E-06	2.33E-05	7.97E-06	1.50E-05	1.67E-05	6.59E-05	1.85E-05	8.31E-06	4.94E-06
Cd	2.11E-06	2.26E-06	8.66E-06	1.18E-05	5.50E-04	1.17E-06	1.40E-06	1.83E-06	7.14E-07	4.66E-06	1.17E-06	1.17E-06	1.00E-06	2.29E-07	0.00E+00
min	2.11E-06	2.26E-06	0.00E+00	7.69E-06	1.69E-04	1.17E-06	1.40E-06	1.83E-06	7.14E-07	4.66E-06	1.17E-06	1.17E-06	1.00E-06	2.29E-07	0.00E+00
max	1.58E-03	1.02E-02	1.85E-03	1.81E-03	2.58E-02	1.90E-03	1.16E-03	1.15E-03	1.36E-03	3.13E-03	5.46E-02	1.64E-03	1.05E-03	1.89E-03	2.93E-03
average	4.49E-04	1.78E-03	4.23E-04	4.37E-04	3.64E-03	3.87E-04	2.28E-04	1.96E-04	4.21E-04	5.91E-04	7.22E-03	4.29E-04	2.94E-04	3.97E-04	5.49E-04

Table S8. The calculated Hazard Quotient (HQ) for all studied heavy metals, in the case of children

HQ	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Cu	7.47E-01	1.80E+00	1.37E+00	1.03E+00	1.62E+00	5.31E-01	7.85E-01	1.16E-01	1.00E+00	1.63E+00	2.53E+00	1.18E+00	6.08E-01	8.71E-01	5.21E-01
Fe	7.20E-03	6.35E-03	9.26E-03	6.28E-03	8.02E-03	4.34E-03	5.78E-03	5.75E-03	6.81E-03	5.53E-03	3.84E-03	6.90E-03	5.24E-03	9.46E-03	6.37E-03
Mn	5.97E-03	5.89E-02	7.92E-04	1.56E-03	6.10E-03	1.02E-03	6.62E-04	7.84E-04	3.08E-02	2.51E-03	4.71E-02	7.41E-04	2.22E-04	7.14E-03	7.87E-04
Zn	1.85E-02	1.19E-01	1.05E-02	2.11E-02	3.00E-01	2.21E-02	4.42E-03	2.37E-03	4.42E-03	3.65E-02	6.37E-01	1.91E-02	1.17E-02	7.46E-03	3.41E-02
Cr	2.47E-04	2.90E-04	7.50E-04	2.42E-04	3.95E-04	2.11E-04	2.45E-04	2.32E-04	3.65E-04	1.26E-04	2.65E-04	2.28E-04	3.31E-04	2.99E-04	8.61E-05
Ni	1.66E-02	9.24E-03	1.35E-02	1.65E-02	3.33E-02	2.07E-02	6.52E-03	7.99E-03	1.55E-02	1.41E-02	7.43E-03	8.49E-03	8.04E-03	1.74E-02	8.18E-03
Pb	1.27E-02	6.75E-03	0.00E+00	6.73E-03	3.00E-01	7.23E-03	6.50E-03	2.04E-02	6.98E-03	1.32E-02	1.47E-02	5.77E-02	1.62E-02	7.28E-03	4.33E-03
Cd	7.37E-06	7.87E-06	3.02E-05	4.10E-05	1.92E-03	4.08E-06	4.88E-06	6.37E-06	2.49E-06	1.62E-05	4.08E-06	4.08E-06	3.49E-06	7.97E-07	0.00E+00
min	7.40E-06	7.90E-06	0.00E+00	2.69E-05	5.93E-04	4.10E-06	4.90E-06	6.40E-06	2.50E-06	1.63E-05	4.10E-06	4.10E-06	3.50E-06	8.00E-07	0.00E+00
max	5.55E-03	3.56E-02	6.48E-03	6.33E-03	9.01E-02	6.64E-03	4.04E-03	4.03E-03	4.77E-03	1.10E-02	1.91E-01	5.73E-03	3.67E-03	6.62E-03	1.02E-02
average	1.57E-03	6.23E-03	1.48E-03	1.53E-03	1.27E-02	1.36E-03	7.98E-04	6.87E-04	1.48E-03	2.07E-03	2.53E-02	1.50E-03	1.03E-03	1.39E-03	1.92E-03

Table S9. The calculated Hazard Quotient (HQ) for all studied heavy metals, in the case of adults

HQ	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Cu	2.13E-01	5.14E-01	3.91E-01	2.95E-01	4.62E-01	1.52E-01	2.24E-01	3.33E-02	2.86E-01	4.67E-01	7.23E-01	3.36E-01	1.74E-01	2.49E-01	1.49E-01
Fe	2.06E-03	1.82E-03	2.65E-03	1.79E-03	2.29E-03	1.24E-03	1.65E-03	1.64E-03	1.95E-03	1.58E-03	1.10E-03	1.97E-03	1.50E-03	2.70E-03	1.82E-03
Mn	1.70E-03	1.68E-02	2.26E-04	4.44E-04	1.74E-03	2.91E-04	1.89E-04	2.24E-04	8.81E-03	7.18E-04	1.35E-02	2.12E-04	6.35E-05	2.04E-03	2.25E-04
Zn	5.28E-03	3.39E-02	2.99E-03	6.03E-03	8.58E-02	6.32E-03	1.26E-03	6.76E-04	1.26E-03	1.04E-02	1.82E-01	5.46E-03	3.33E-03	2.13E-03	9.76E-03
Cr	7.07E-05	8.27E-05	2.14E-04	6.92E-05	1.13E-04	6.02E-05	7.00E-05	6.64E-05	1.04E-04	3.60E-05	7.57E-05	6.53E-05	9.45E-05	8.55E-05	2.46E-05
Ni	4.73E-03	2.64E-03	3.84E-03	4.70E-03	9.50E-03	5.91E-03	1.86E-03	2.28E-03	4.43E-03	4.04E-03	2.12E-03	2.42E-03	2.30E-03	4.97E-03	2.34E-03
Pb	3.63E-03	1.93E-03	0.00E+00	1.92E-03	8.58E-02	2.06E-03	1.86E-03	5.81E-03	1.99E-03	3.76E-03	4.19E-03	1.65E-02	4.63E-03	2.08E-03	1.24E-03
Cd	2.11E-06	2.25E-06	8.62E-06	1.17E-05	5.48E-04	1.17E-06	1.39E-06	1.82E-06	7.11E-07	4.64E-06	1.17E-06	1.17E-06	9.96E-07	2.28E-07	0.00E+00
min	2.11E-06	2.25E-06	0.00E+00	1.17E-05	1.13E-04	1.17E-06	1.39E-06	1.82E-06	7.11E-07	4.64E-06	1.17E-06	1.17E-06	9.96E-07	2.28E-07	0.00E+00
max	2.13E-01	5.14E-01	3.91E-01	2.95E-01	4.62E-01	1.52E-01	2.24E-01	3.33E-02	2.86E-01	4.67E-01	7.23E-01	3.36E-01	1.74E-01	2.49E-01	1.49E-01
average	2.88E-02	7.14E-02	5.01E-02	3.87E-02	8.10E-02	2.10E-02	2.89E-02	5.50E-03	3.80E-02	6.09E-02	1.16E-01	4.54E-02	2.32E-02	3.29E-02	2.05E-02