

## ASSESSING THE CHEMICAL COMPOSITION OF NATURAL WATER USING ANALYTICAL CHEMISTRY TECHNIQUES. A CASE STUDY IN THE ORHEI DISTRICT, REPUBLIC OF MOLDOVA

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Table S1

**Quality parameters (LN, LD, U) and coefficients of the calibration curves.**

No.	El.	$\lambda$ , nm	LN	a	b	R <sup>2</sup>	LD	U, %
1.	Ag	328.068	20 ÷ 1000 µg(Ag)/L	-0.003094	0.198056	0.980405	7.4 µg(Ag)/L	0.0037
2.	Al	394.401	20 ÷ 2000 µg(Al)/L	0.012461	4.085172	0.987818	2.2 µg(Al)/L	0.147
3.	Al	396.152	20 ÷ 2000 µg(Al)/L	0.151051	8.196791	0.986330	1.3 µg(Al)/L	0.165
4.	As	189.042	20 ÷ 6000 µg(As)/L	-0.027719	2.224936	0.998300	1.7 µg(As)/L	0.050
5.	As	193.759	20 ÷ 6000 µg(As)/L	-0.030333	1.717150	0.998320	2.0 µg(As)/L	0.038
6.	B	208.893	100 ÷ 7000 µg(B)/L	0.002383	0.100393	0.995166	21 µg(B)/L	0.0037
7.	Ba	413.066	5 ÷ 12000 µg(Ba)/L	-0.242547	8.084276	0.998536	1.0 µg(Ba)/L	0.135
8.	Be	249.473	400 ÷ 11000 µg(Be)/L	-0.002844	0.437853	0.998291	8.7 µg(Be)/L	0.0078
9.	Bi	190.234	200 ÷ 1000 µg(Bi)/L	-0.006843	1.263806	0.982045	2.9 µg(Bi)/L	0.023
10.	Bi	223.061	200 ÷ 1000 µg(Bi)/L	-0.016926	1.186784	0.980056	1.4 µg(Bi)/L	0.023
11.	Ca	315.887	0.4 ÷ 151 mg(Ca)/L	0.004169	0.073784	0.999672	0.011 mg(Ca)/L	0.0041
12.	Ca	317.933	0.4 ÷ 151 mg(Ca)/L	0.015403	0.239463	0.999699	0.005 mg(Ca)/L	0.013
13.	Cd	214.438	10 ÷ 2000 µg(Cd)/L	-0.377000	36.026849	0.988548	0.04 µg(Cd)/L	0.663
14.	Cd	226.502	10 ÷ 2000 µg(Cd)/L	-0.227424	21.760364	0.988647	0.07 µg(Cd)/L	0.399
15.	Co	228.616	200 ÷ 2000 µg(Co)/L	-0.133010	12.202615	0.988997	0.15 µg(Co)/L	0.220
16.	Cr	267.716	200 ÷ 2000 µg(Cr)/L	-0.007433	1.049621	0.986694	3.3 µg(Cr)/L	0.021
17.	Cu	324.754	200 ÷ 2000 µg(Cu)/L	-0.000666	0.223818	0.990590	3.7 µg(Cu)/L	0.0037
18.	Fe	259.837	200 ÷ 2000 µg(Fe)/L	0.003318	0.348624	0.965969	9.1 µg(Fe)/L	0.011
19.	Fe	259.940	200 ÷ 2000 µg(Fe)/L	0.018510	1.075736	0.987487	3.1 µg(Fe)/L	0.021
20.	Ga	294.364	200 ÷ 1000 µg(Ga)/L	-0.001035	0.177936	0.985882	29.5 µg(Ga)/L	0.0028
21.	Ge	265.118	20 ÷ 5000 µg(Ge)/L	0.003974	0.183550	0.999697	21.1 µg(Ge)/L	0.0017
22.	Hg	194.227	5 ÷ 5000 µg(Hg)/L	-0.001404	2.920979	0.999564	0.9 µg(Hg)/L	0.018
23.	In	230.606	200 ÷ 1000 µg(In)/L	-0.008263	1.020557	0.980816	2.0 µg(In)/L	0.019
24.	K	766.490	0.4 ÷ 151 mg(K)/L	1.062601	4.405862	0.999603	0.270 mg(K)/L	0.269
25.	K	769.896	0.4 ÷ 151 mg(K)/L	3.703524	1.929445	0.999771	0.010 mg(K)/L	0.397
26.	Li	670.784	400 ÷ 12000 µg(Li)/L	-0.936198	91.352181	0.997945	0.2 µg(Li)/L	1.808
27.	Mg	279.079	0.4 ÷ 151 mg(Mg)/L	-0.001171	0.142021	0.998542	0.024 mg(Mg)/L	0.011
28.	Mn	257.610	200 ÷ 2000 µg(Mn)/L	-0.070475	7.064890	0.986828	0.5 µg(Mn)/L	0.140
29.	Mo	202.030	5 ÷ 1000 µg(Mo)/L	-0.006487	13.221700	0.999208	0.3 µg(Mo)/L	0.050

Continuauion of Table S1

30.	Na	818.326	2.02 ÷ 151 mg(Na)/L	-0.608142	0.577645	0.999775	0.025 mg(Na)/L	0.253
31.	Ni	231.604	200 ÷ 2000 µg(Ni)/L	-0.072413	7.698131	0.990465	0.2 µg(Ni)/L	0.129
32.	P	213.618	70 ÷ 5000 µg(P)/L	0.018411	0.689026	0.991559	1.3 µg(P)/L	0.030
33.	Pb	220.353	200 ÷ 2000 µg(Pb)/L	-0.017846	2.180200	0.979221	0.8 µg(Pb)/L	0.054
34.	S	182.034	400 ÷ 6000 µg(S)/L	0.036917	0.568722	0.996727	5.5 µg(S)/L	0.018
35.	Sb	206.833	15 ÷ 6000 µg(Sb)/L	0.008032	2.979985	0.999042	1.8 µg(Sb)/L	0.038
36.	Sb	217.581	15 ÷ 6000 µg(Sb)/L	0.002587	0.779267	0.998736	1.5 µg(Sb)/L	0.011
37.	Se	196.090	10 ÷ 1000 µg(Se)/L	0.005470	2.794951	0.990104	1.4 µg(Se)/L	0.030
38.	Sn	189.989	15 ÷ 5000 µg(Sn)/L	0.018305	6.259499	0.999997	0.5 µg(Sn)/L	0.0047
39.	Sr	346.446	0.4 ÷ 151 mg(Sr)/L	-0.004574	0.200373	0.999897	0.008 mg(Sr)/L	0.0062
40.	Te	214.281	30 ÷ 6000 µg(Te)/L	-0.011604	1.087623	0.998260	1.4 µg(Te)/L	0.025
41.	Ti	308.802	10 ÷ 1000 µg(Ti)/L	0.000287	0.387340	0.999801	3.1 µg(Ti)/L	0.0007
42.	Ti	334.941	10 ÷ 1000 µg(Ti)/L	0.001365	0.484439	0.999892	2.1 µg(Ti)/L	0.0007
43.	Tl	190.856	200 ÷ 1000 µg(Tl)/L	-0.025241	1.624193	0.981182	1.9 µg(Tl)/L	0.030
44.	V	292.402	200 ÷ 2000 µg(V)/L	-0.015507	1.910304	0.986529	3.2 µg(V)/L	0.038
45.	Zn	206.200	200 ÷ 2000 µg(Zn)/L	-0.137844	17.107746	0.989608	0.17 µg(Zn)/L	0.300
46.	Zn	213.856	200 ÷ 2000 µg(Zn)/L	-0.107842	13.031004	0.986743	0.09 µg(Zn)/L	0.258

Table S2

**Details about reference standards and internal standard (IS) used in ICP-OES spectrometry applications.**

Type of standard	Details of standards
Reference standards	Alkali metal mix for ICP; TraceCERT®, Li, Na, K, Rb and Cs, 100 mg/L. Sigma-Aldrich, Cod: 96441-100ML; Lot: BCCC2487
	Alkaline earth metal mix for ICP; TraceCERT®, Be, Mg, Ca, Sr and Ba, 100 mg/L. Sigma-Aldrich, Cod: 67288-100ML; Lot: BCBZ8697
	Periodic table mix 1 for ICP; TraceCERT®, 33 elements, 10 mg/L in nitric acid: Al, As, Ba, Be, Bi, B, Ca, Cd, Cs, Cr, Co, Cu, Ga, In, Fe, Pb, Li, Mg, Mn, Ni, P, K, Rb, Se, Si, Ag, Na, Sr, S, Te, Tl, V and Zn in 10% nitric acid (contains HF traces). Merck, Sigma-Aldrich, Supelco®, Cod: 92091-100ML, Lot: BCCB9855
	Multielement Standard Solution 6 for ICP; TraceCERT®, 23 elements, 100 mg/L each in nitric acid and hydrofluoric acid: Al, Sb, Ba, Pb, B, Ca, Cd, Cr, Co, Fe, K, Cu, Li, Mg, Mn, Mo, Na, Ni, P, Si, Ti, V and Zn. Merck, Sigma-Aldrich, Supelco®, Cod: 43843-100ML, Lot: BCCF4114
	Metalloid and non-metal mix for ICP; TraceCERT®, 10 elements, 100 mg/L each in nitric acid and hydrofluoric acid: B, Si, P, S, Ge, As, Se, Sn, Sb and Te. Merck, Sigma-Aldrich, Supelco®, Cod: 55263-100ML, Lot: BCBZ8058
	Mercury Standard for ICP, TraceCERT®, 1 g/L Hg in nitric acid. Merck, Sigma-Aldrich, Supelco®, Cod: 28941-100ML, Lot: 28941
Internal standard	Scandium Standard for ICP, TraceCERT®, 10 g/L Sc in nitric acid 10000 mg(Sc)/L. Merck, Sigma-Aldrich, Supelco®, Cod: 92504-100ML, Lot: BCCF1932

**Elemental composition of samples analysed using ICP-OES.**

<i>No.</i>	<i>Element</i>	<i>Sample No. 1 / Concentration</i>	<i>Unit of meas.</i>
1.	Ag	19.8±1.0	µg/L
2.	Al	77±11	µg/L
3.	As	19.1±1.4	µg/L
4.	B	0.92±0.01	mg/L
5.	Ba	0.073±0.002	mg/L
6.	Be	<8.7	µg/L
7.	Bi	16±2	µg/L
8.	Ca	91±1	mg/L
9.	Cd	10.5±0.1	µg/L
10.	Co	11±0.1	µg/L
11.	Cr	6.3±1.0	µg/L
12.	Cu	0.014±0.003	mg/L
13.	Fe	<0.005	mg/L
14.	Ga	32±10	µg/L
15.	Ge	<20	µg/L
16.	Hg	<0.5	µg/L
17.	In	14±0.5	µg/L
18.	K	17.5±0.5	mg/L
19.	Li	0.124±0.007	mg/L
20.	Mg	108.7±1.5	mg/L
21.	Mn	18±0.2	µg/L
22.	Mo	5.6±0.2	µg/L
23.	Na	334±9.7	mg/L
24.	Ni	14±0.1	µg/L
25.	P	71±9	µg/L
26.	Pb	12.2±0.6	µg/L
27.	S	280±5.8	mg/L
28.	Sb	<1	µg/L
29.	Se	3.9±1.0	µg/L
30.	Sn	5±0.1	µg/L
31.	Sr	4.240±0.04	mg/L
32.	Te	10±0.5	µg/L
33.	Ti	<3.1	µg/L
34.	Tl	9±0.5	µg/L
35.	V	10±3	µg/L
36.	Zn	10±0.2	µg/L