Table S1. (Denmark): number of chemical analyses for each element (n), account of LODs in the dataset, range of LODs, the number and percentage of analyses < LOD, the max substitute value and the number of analyses with the max substituted.

Element	unit	No of analyses (n)	< LOD (n)	< LOD (%)	LOD range (min-max)	max substitute concentration	n
As	µg/l	17935	1491	8.3	0.01-1.0	1.5	1
Cd	µg/l	660	559	84.7	0.003-0.5	0.75	1
Cr	µg/l	454	245	54.0	0.01-0.5	0.75	5
Cu	µg/l	616	206	33.4	0.03-5.0	7.5	1
Ni	µg/l	18906	3487	18.4	0.02-3.0	4.5	222
Zn	µg/l	622	197	31.7	0.3-10.0	15	1
F	mg/l	17100	1132	6.6	0.02-0.5	0.75	6
SO$_4$	mg/l	17977	404	2.2	0.2-1.5	2.25	4
O$_2$	mg/l	18975	3464	18.3	0.01-2.0	6	1
NO$_3$	mg/l	17822	12666	71.1	0.002-1.0	1.5	323
Fe	mg/l	17902	1136	6.3	0.0002-0.02	0.03	1

Table S2. (Serbia): number of chemical analyses for each element (n), account of LODs in the dataset and percentage of analyses < LOD, the max substitute value and max LOD substituted.

Element	Unit	n	<LOD (n)	<LOD (%)	LOD max
As	µg/l	132	15	11%	4
Cd	µg/l	130	31	24%	0.04
Cr	µg/l	132	25	19%	0.4
Cu	µg/l	132	19	14%	1.62
Ni	µg/l	130	26	20%	2
Zn	µg/l	124	6	5%	1
F	mg/l	132	3	2%	0.1
SO$_4$	mg/l	132	7	5%	
NO$_3$	mg/l	132	1	1%	

Table S3. (Slovenia): number of chemical analyses for each element, account of LOQs in the dataset (two were reported in 2016), range of LOQs, the number and percentage of analyses < LOQ, the max substitute value and the number of analyses with the max substitute.

	No. of analyses without anthropogenic influence	No. of analyses with anthropogenic influence	Low LOQ	% samples below low LOQ	High LOQ	% samples below high LOQ	% of samples below LOQ	max LOQ/2
As (µg/L)	86	92	<0.1	7	<1	56	63	0.5
Cd (µg/L)	87	91	<0.01	31	<0.02	40	71	0.01
Cr (µg/L)	87	91	<0.4	31	<1	22	53	0.5
Cu (µg/L)	87	92	<0.1	4	<1	41	45	0.5
F (mg/L)	83	92	<0.04	18	<0.2	46	64	0.1
Fe (mg/L)	86	92	<0.04	35	<0.1	43	79	0.05
Ni (µg/L)	87	92	<0.1	13	<1	26	38	0.5
Zn (µg/L)	87	92	<9	35	<10	39	74	5
SO$_4$ (mg/l)	83	92	nd	0	nd	0	0	/
NO$_3$ (mg/L)	87	92			<2.2	4	4	1.1

Table S4. (Loire-Bretagne, France): number of chemical analyses for each element (n), account of value > LOQs in the dataset, range of LOQs (Low, high), percentage of analyses < LOQ, with high LOQ, the maximum value substituted

Element	All (n)	No of analysis > LOQ	low LOQ	high LOQ	< LOQ (%)
As (µg/l)	16041	7283	0.005	1.5	55%
Cd (µg/l)	3656	3187	0.5	0.5	13%
Cr (µg/l)	9928	5453	0	1.25	45%

Cu (µg/l)	17373	2920	0.005	1	**83%**
Fe (µg/l)	26361	11971	0	50	55%
Ni (µg/l)	4111	1694	0.025	1	59%
Zn (µg/l)	4378	3225	0.05	5	26%
F (mg/l)	10316	7527	0.005	5	27%
SO$_4$ (mg/l)	29998	29021	0.05	2.5	3%
NO$_3$ (mg/l)	48554	43142	0.05	2.5	11%

Table S5. (Internal basins, Catalonia): Number of analyses for each element (n) and number and percentage of analyses < LOD, range of LOD and maximum value imputed, with each method.

*lrEM: "Log-Ratio EM Algorithm" method with the lrEM function for R-studio software (package [zCompositions v1.3.4].

Element	unit	All (n)	< LOD (n)	< LOD (%)	LOD range (min-max)	max substitute concentration lrEM*	max substitute concentration LOD/2
As	µg/L	2458	784	31.90	0.01 - 1	0.74	0.5
Cd	µg/L	7061	6554	92.82	-	-	
Cu	µg/L	8243	2677	32.48	0.5 - 10	4.13	2.5
Cr	µg/L	8162	6862	84.07	1 - 5	-	
Fe	µg/L	5963	2131	35.74	5 - 50	-	
Ni	µg/L	7077	4061	57.38	1 - 5	-	
Zn	µg/L	7322	1746	23.85	0.1 - 5	2.59	2
SO$_4$	mg/l	8301	66	0.80	8 - 10	8.66	4
NO3	mg/l	8356	1252	14.98	0.1 - 5	3.16	2.5

Table S6. (Austria): Dataset overview, ranked by percentage of values below LOD or LOQ.

Parameter	Number of value below LOD or LOQ	Number of analysis (n)	% of values below LOD or LOQ	Max. LOD or LOQ (mg L^{-1})	Min. LOD or LOQ (mg L^{-1})
As	21750	28040	77,57	0,001	1,16E-04
Cd	27062	28037	96,52	0,0001	1,34E-05
Cl	3750	43752	8,57	1	0,14
Cr	23452	28039	83,64	0,001	8,00E-05
Cu	15054	28038	53,69	0,005	7,00E-05
Fe	29049	43742	66,41	0,02	2,70E-04
Ni	21632	28042	77,14	0,001	3,00E-05
Zn	7575	28041	27,01	0,02	1,84E-04
SO$_4$	328	43729	0,75	1	0,2
NO$_3$	3028	43767	6,92	1	0,14

Table S7. (Spain, DRB): Number and percentage of chemical analyses below the limit of quantification (LOQ), range of LOQs in the dataset and min and max substituted value.

Element	unit	Number of values < LOQ	Period with records	< LOQ (n)	< LOQ (%)	LOQ range (min-max)	Min	Max
As	µg/l	4234	10-20	2642	62.40	0.1-5	0.102	801
Cd	µg/l	4456	11-20	3918	87.92	0.02-1	0.02	78
Cr	µg/l	807	11-13	279	34.57	1	1	28
Cu	µg/l	4332	10-20	2474	57.11	1-6	1	3590
Ni	µg/l	799	11-13	646	80.85	1-7	0.59	19
Zn	µg/l	1328	10-16	535	40.2	0.002-0.06	0.002	6.06
F	mg/l	3783	10-20	1318	34.84	0.05-0.5	0.01	8.85
Cl	mg/l	6457	10-20	486	7.5	1-10	0.22	1152
SO$_4$	mg/l	6341	10-20	908	14.65	1-10	1	2822.2
O$_2$	mg/l	3091	10-20	-	-	-	0.04	17.4
NO$_3$	mg/l	6341	10-20	1317	20.77	0.15-5	0.21	1105

Table S8. (Loire-Bretagne, France): Number of water sampling points with data for each element and each group of prevailing pressure.

Element	No sampling points	Agriculture (CLC)		Natural area (CLC)		Urban area (CLC)		Pollution point source (BASIAS)		Mining and mineralization	
As	3512	2007	57%	1303	37%	202	6%	993	28%	442	13%
Zn	495	353	71%	93	19%	49	10%	182	37%	54	11%
Ni	2362	1413	60%	823	35%	126	5%	766	32%	458	19%
Cd	3708	2111	57%	1394	38%	203	5%	1056	28%	458	12%
Cr	426	294	69%	88	21%	44	10%	155	36%	59	14%
Cu	435	304	70%	86	20%	45	10%	159	37%	54	12%
F	3313	1953	59%	1160	35%	200	6%	974	29%	367	11%
SO4	3783	2152	57%	1427	38%	204	5%	1081	29%	470	12%

Table S9. (Denmark): Number of water sampling points with data for each element and each group of prevailing pressure and results from the Kruskal-Wallis rank sum test.

Element	all	Prevailing pressures										Kruskal-Wallis rank sum test
		agricultural		industrial		mining		urban		no or other		
	n	n	%	n	%	n	%	n	%	n	%	
As	6352	5447	85.8	45	0.7	2	0.03	796	12.5	62	0.98	Significant ($p < 0.05$)
Cd	356	287	80.6	17	4.8			52	14.6			Significant ($p < 0.05$)
Cr	250	187	74.8	7	2.8			56	22.4			Significant ($p < 0.05$)
Cu	289	217	75.1	7	2.4			64	22.1	1	0.35	Significant ($p < 0.05$)
Ni	6358	5452	85.8	45	0.7	2	0.03	797	12.5	62	0.98	Significant ($p < 0.05$)
Zn	363	281	77.4	19	5.2		0	62	17.1	1	0.28	Not significantly different
F	6349	5444	85.7	45	0.7	2	0.03	796	12.5	62	0.98	Significant ($p < 0.05$)
SO4	6360	5454	85.8	45	0.7	2	0.03	797	12.5	62	0.97	Significant ($p < 0.05$)

Table S10. (Spain, DRB): Number of water sampling points with data for each element and each group of prevailing pressure and results from the Kruskal-Wallis rank sum test

Element	all	agricultural		no or other		Kruskal-Wallis rank sum test
	n	n	%	n	%	
As	460	358	22.17	102	77.82	Not significant ($p > 0.05$)
Cd	449	353	21.38	96	78.62	Not significant ($p < 0.05$)
Cu	461	358	22.34	103	77.66	Not significant ($p < 0.05$)
F	440	338	76.82	102	23.18	Significant ($p < 0.05$)**
SO4	465	361	77.63	104	22.36	Significant ($p < 0.05$)**

Table S11. (Austria): confusion matrix for lithology

from / to	Metamorphic rocks	Sedimentary: clays and/ or marls	Sedimentary: gravel	Sedimentary: others	True classification (n)	% correct prediction
Metamorphic rocks	45	0	8	0	53	85%
Sedimentary: clays and/or marls	3	9	145	2	159	6%
Sedimentary: gravel	207	21	911	29	1168	78%
Sedimentary: other	135	2	61	0	198	0%
Total	390	32	1125	31	1578	61%

Table S12. (Denmark): Natural background levels (NBL) for sedimentary aquifers combined with pH & redox conditions.

HOVER-lithology	Elements	units	HOVER-pH	NBLs per water family				NBLs (only lithology)
				HOVER-redox				
				A	B	C & D	X	

HOVER-lithology	Elements	units	HOVER-pH					NBLs (only lithology)
Sands	As	µg/l	Acidic	NA	NA	3	NA	6.8
			Basic	2.3	NA	5.6	3.6	
			Neutral	1.3	NA	9.6	3.8	
	Ni	µg/l	Acidic	NA	NA	4.7	NA	1.8
			Basic	1.3	NA	1	1.4	
			Neutral	2.2	NA	1.3	3.4	
	SO4	mg/l	Acidic	NA	NA	87	NA	87
			Basic	68	NA	74	86	
			Neutral	86	NA	89	111	
	F	mg/l	Acidic	NA	NA	0.7	NA	0.4
			Basic	0.2	0.2	0.3	0.2	
			Neutral	0.3	NA	0.4	0.3	
Carbonates	As	µg/l	Basic	2.2	NA	4	3.3	3.9
			Neutral	2	2.7	4.7	7.7	
	Ni	µg/l	Basic	4	NA	2.1	3.2	5.3
			Neutral	12	20	3	7.7	
	SO4	mg/l	Basic	43	NA	63	48	89
			Neutral	92	100	89	82	
	F	mg/l	Basic	0.3	NA	0.9	1.3	1.2
			Neutral	0.4	0.8	1.2	1.7	

Table S13. (Loire-Bretagne, France) Natural background levels (NBL) for the sedimentary aquifers combined with pH & redox conditions.

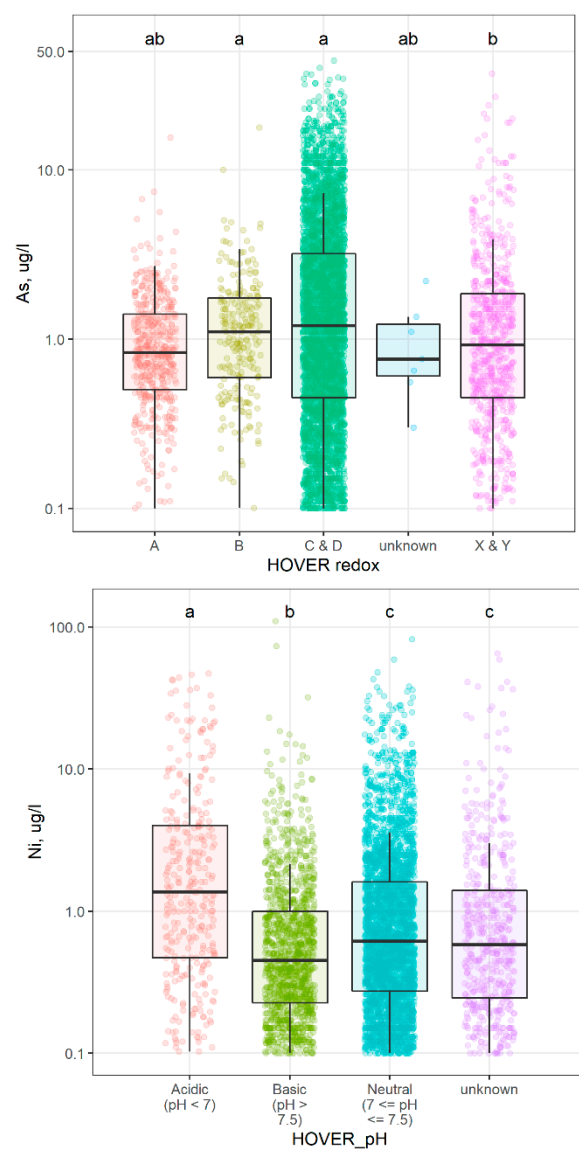| HOVER-lithology	Elements	units	HOVER-pH	NBLs per water family			NBLs (only lithology)
				HOVER-redox			
				A & B	C&D	All redox	
Sands	As	µg/l	All pH	1.1	1.5		1.46
	Ni	µg/l	Acidic	10.2	13.5		2.3
			Basic	1.3	2.6		
			Neutral	2.1	2.3		
	Zn	µg/l	Acidic			16.6	12.3
			Basic			11.8	
			Neutral			10	
	Cu	µg/l	Acidic	8			4.4
			Basic		1.3		
			Neutral	8.8	3.5		
Carbonates	As	µg/l		1.2	6.4		3
	Ni	µg/l	Acidic				2.8
			Basic	3.5	0.6		
			Neutral	2.2	5.5		
	Cu	µg/l	Basic	2.2	0.3		
			Neutral	3.2	0.6		

Figure S.1.. Boxplots showing the variation of As and Ni concentrations in the Danish dataset for different pH and redox classes. The categories sharing letters (above the boxplot) are not significantly different at the 95% confidence level based on the post-hoc Nemenyi test [56].