

Supporting Information

Pb and Fe flow through the mire-lake complex of Skogaryd catchment - a system under anthropogenic influence

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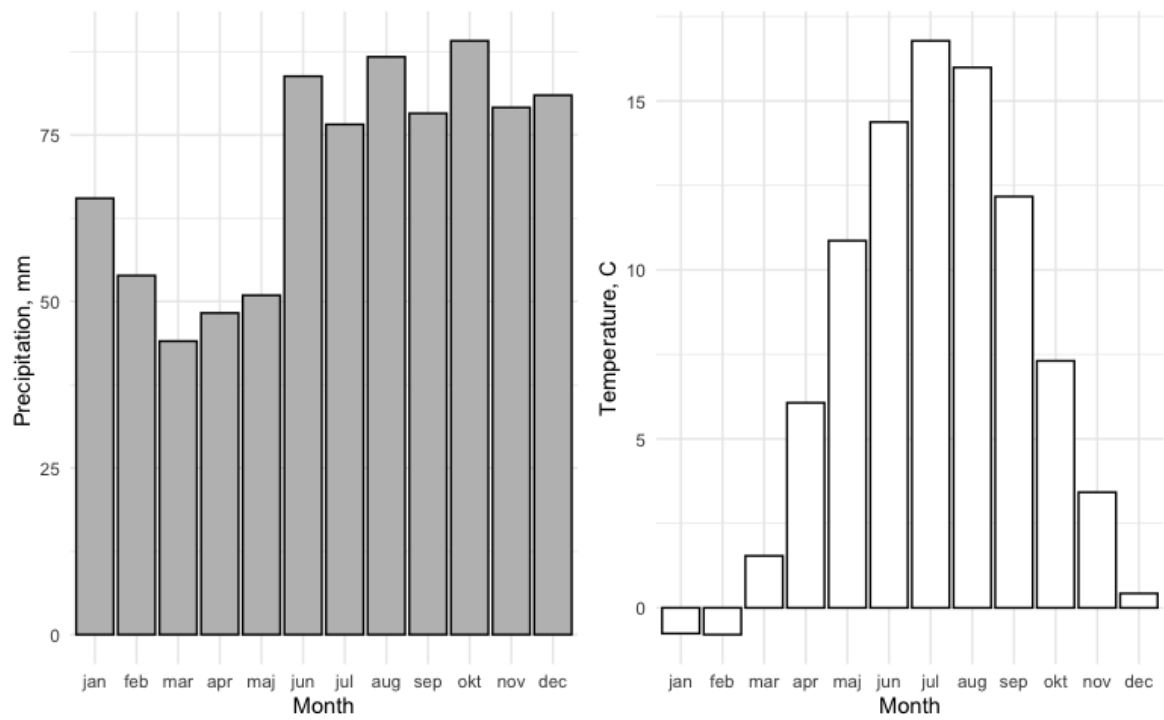


Fig S1. Monthly total precipitation and average temperature for the climate normal period 1991-2020 at the meteorological station in Vänersborg ~10km east of Mycklemossen (Swedish Meteorological and Hydrological Institute).

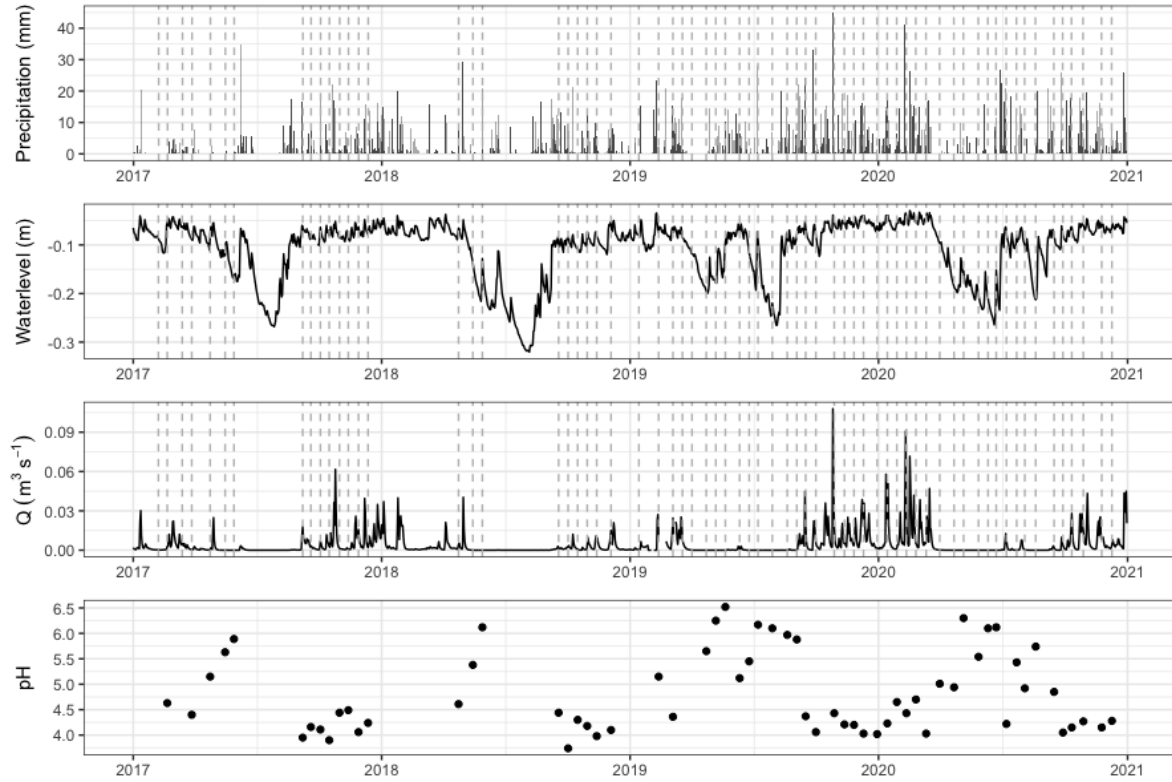


Fig S2. Daily total precipitation and average water table in Mycklemossen and average discharge and pH in stream water from Mycklemosse. Vertical dotted lines mark grab sampling events in stream water (S1) from Mycklemossen where pH (and DOC, metal concentrations) was measured.

Table S1. Average element concentration (mg/kg) in peat cores of Mycklemossen mire at selected depth intervals (n=5) in 3 micro topography types (Type): Hollow (HOL), hummock (HUM) and an intermediate form (INT).

Element	Tope	15-20 cm		20-25 cm		25-50 cm		120-125 cm		420-425 cm	
		mean	se	mean	se	mean	se	mean	se	mean	se
Arsenic	HOL	2.26	± 0.42	1.98	± 0.41	1.51	± 0.39	0.58	± 0.18	3.56	± 1.21
	HUM	1.52	± 0.64	2.26	± 0.98	3.75	± 1.26	0.54	± 0.07	2.43	± 0.54
	INT	3.69	± 0.91	3.40	± 0.77	3.23	± 0.85	0.50	± 0.09	3.65	± 1.15
Lead	HOL	32.21	± 8.64	22.17	± 5.79	14.89	± 4.65	4.75	± 2.04	1.75	± 0.53
	HUM	28.26	± 10.80	46.49	± 18.89	91.80	± 33.71	7.60	± 2.45	3.07	± 1.76
	INT	64.25	± 17.23	60.38	± 26.08	58.50	± 27.79	5.19	± 1.14	3.15	± 1.20
Cadmium	HOL	0.47	± 0.06	0.40	± 0.08	0.30	± 0.09	0.06	± 0.02	0.14	± 0.04
	HUM	1.64	± 0.45	2.52	± 0.86	2.22	± 0.83	0.11	± 0.05	0.07	± 0.01
	INT	0.91	± 0.11	0.70	± 0.13	0.60	± 0.12	0.06	± 0.01	0.11	± 0.02
Chromium	HOL	2.44	± 0.57	5.14	± 3.19	1.47	± 0.11	8.17	± 6.93	4.37	± 2.63
	HUM	7.55	± 2.14	11.59	± 6.84	16.62	± 3.35	6.01	± 4.97	14.63	± 9.47
	INT	12.07	± 5.92	16.80	± 6.05	7.60	± 4.37	18.70	± 14.56	7.80	± 3.57
Iron	HOL	606.23	± 119.63	641.77	± 152.07	610.21	± 132.26	1433.99	± 247.94	7147.57	± 1017.80
	HUM	1237.04	± 423.68	1532.24	± 568.03	1757.24	± 435.70	1413.89	± 622.78	8481.66	± 2261.55
	INT	1130.62	± 399.66	856.25	± 222.24	817.74	± 237.26	1476.65	± 599.08	7457.85	± 768.39

Table S2: ICP-MS parameters for determination of Pb isotopic analysis.

Laboratory and Sample Preparation	
Laboratory name	Microgeochemistry Laboratory, University of Gothenburg
Sample type	surface water samples
Sample preparation	acidified to 2% HNO ₃
Measurement session	240912
Autosampler and Sample Uptake	
Model and type	ASX-500
Uptake speed (Nebulizer Pump) [rps]	0.1
ICP-MS Instrument	
Make, Model and type	Agilent 8800QQQ
Sample introduction	MicoMist Nebulizer
Spraychamber Temp [C]	2
Plasma	
RF power [W]	1550
RF matching [V]	1.8
Sample depth [mm]	8
Nebulizer gas flow [l/min]	1.07
Lenses	
Extract 1 [V]	4.1
Extract 2 [V]	-200
Omega bias [V]	-95
Omega lens [V]	7.8
Q1 entrance [V]	2
Q1 exit [V]	-2
Cell focus [V]	1
Cell entrance [V]	-81
Cell exit [V]	-85
Deflect [V]	5.8
Plate bias [V]	-71
Q1	
Q1 bias [V]	-2
Q1 prefilter bias [V]	-32
Q1 postfilter bias [V]	-22
Cell	
reaction gas	N ₂ O

reaction gas flow	22%
OctP bias [V]	-5.1
OctP RF [V]	200
Energy discrimination [V]	-5.2

Q2	
QP Bias	-10.3

Table S3: ICP-MS acquisition parameters for Pb isotopic analysis

Acq Mode	Spectrum		
Q2 Peak Pattern	3 points		
Replicates	10		
Sweeps/Replicate	250		
Stabilization time	15 s		
Wait Time Offset	2 ms		
Element	Q1	Q2	Dwell time
	(m/z)	(m/z)	(s)
Hg	202	202	1.5
Pb+Hg	204	204	20
Pb	206	206	3.0
Pb	207	207	3.0
Pb	208	208	1.5
PeriPump Settings			
Pre Run			
Uptake time	40	s	sample (0.5 rps)
Stabilize	30	s	sample (0.5 rps)
Post Run			
Rise Port	10	s	0.5% HNO3 (0.1 rps)
Rise Vial 1	30	s	2 % HNO3 (0.1 rps)
Rise Vial 1	30	s	2 % HNO3 (0.5 rps)
Rise Vial 1	40	s	2 % HNO3 (0.5 rps)

Table S4. Reference material for ICP-MS

			207Pb /206Pb	2s2	208Pb /206Pb	2s2	206Pb/204Pb	2s2	207Pb /204Pb	2s2	208Pb /204Pb	2s2
Primary reference material												
NIST SRM 981	Catanzaro et al (1968)		0.91464	0.00033	2.1681	0.0008	16.937	0.011	15.49	0.01	36.72	0.03
Secondary reference solutions												
NIST SRM 981	approximately 5.5 µg/l Pb	weighted mean	0.9142	0.0001	2.1667	0.0016	16.938	0.013	15.484	0.018	36.626	0.066
		MSWD	0.13		1.3		0.41		0.33		3.5	
		n=	5/5		5/5		5/5		5/5		5/5	
NIST SRM 981	approximately 1.1 µg/l Pb	weighted mean	0.9179	0.0017	2.1723	0.0036	16.907	0.029	15.531	0.033	36.676	0.076
		MSWD	0.49		0.87		0.57		1.14		1.7	
		n=	5/5		5/5		5/5		5/5		5/5	
AQUA-1	Yeghicheyan et al. (2021)		0.8990	0.301	2.144	0.109	17.171	0.008	15.535	0.041	37.03	0.237
	this study	weighted mean	0.955	0.001	2.148	0.003	17.158	0.032	15.533	0.028	36.799	0.066
		MSWD	0.4		0.19		0.99		0.51		0.48	
		n=	5/5		5/5		5/5		5/5		5/5	

Table S5. ^{14}C dating of peat cores sampled at location T3. Peat samples were collected in 20-25, 120-125 and 420-25 cm depth from hummock, intermediate and hollow micro topographies. Values are means of three technical replicates $\pm$ SD. Bomb peak (BP) age is 1950.

Topography	Depth (cm)	Age (yrs BP-age)	Date of origin
Hummock	20-25	NA*	NA*
	120-125	875 $\pm$ 28	1075
	425-450	3 526 $\pm$ 30	1576 (BC)
Intermediate	20-25	59 $\pm$ 28	1891
	120-125	1 839 $\pm$ 29	111
	425-450	3 927 $\pm$ 31	1977 (BC)
Hollow	20-25	256 $\pm$ 28	1694
	120-125	1 105 $\pm$ 29	845
	420-425	3 199 $\pm$ 30	1249 (BC)

* Sample contained too much modern C for accurate dating of sample age.

Table S6. Output from mixed effects models testing the effects of sampling depth and topography type and their interactions on peat bulk density, pore water pH, SOM%, C content, N content, C to N ratio, $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$. There was no effect of depth and type on $\delta^{18}\text{O}$ and the results are not shown. $p < 0.05$ are marked in bold.

	Bulk density ¹			pH			SOM ¹			C% ¹		
	Df	X ²	p	Df	X ²	p	Df	X ²	p	Df	X ²	p
Depth	2	18.6	<0.001	1	.3	<0.001	2	27.9	<0.001	1	23.6	<0.001
Type	2	1.0	0.59	2	4.3	0.12	2	6.7	0.04	2	0.7	0.70
Depth*Type	4	0.8	0.93	2	6.5	0.04	4	5.3	0.26	2	0.9	0.65

	N% ¹			C/N ¹			$\delta^{13}\text{C}$ ¹			$\delta^{15}\text{N}$ ¹		
	Df	X ²	p	Df	X ²	p	Df	X ²	p	Df	X ²	p
Depth	2	27.8	<0.001	2	4	<0.001	2	47.6	<0.001	2	20.4	<0.001
Type	2	2.8	0.25	2	2.0	0.38	2	1.5	0.47	2	2.0	0.36
Depth*Type	4	10.2	0.04	4	0	0.04	4	7.7	0.10	4	1.2	0.89

¹Depth was treated as a quadratic polynomial term

Table S7. Output from mixed effects models testing the effects of sampling depth and topography type and their interactions on peat lead (Pb) and iron (Fe) concentrations. p < 0.05 are marked in bold.

	Df	Pb		Fe	
		X ²	p	X ²	p
Depth	2	31.5	< 0.001	288.9	< 0.001
Type	2	7.4	0.02	3.4	0.18
Depth*Type	4	4.1	0.39	1.1	0.90

Sample locality 01

1	5-101220201	##	6378	114943	98527	235933	61	##	0.04%	1.146	0.003	2.113	0.006	17.89	0.04	15.63	0.03	37.73	0.05
2	5-101220501	##	6821	123014	105523	252162	69	##	0.04%	1.144	0.003	2.111	0.005	17.89	0.04	15.65	0.05	37.70	0.08
3	5-101220801	##	13042	236578	202878	486051	31	##	0.02%	1.146	0.004	2.112	0.006	17.90	0.04	15.62	0.03	37.75	0.06
4	5-101221001	##	10486	189857	163662	391736	45	##	0.02%	1.144	0.003	2.116	0.005	17.89	0.05	15.65	0.05	37.80	0.06
5	5-101221201	##	5894	105892	90861	217062	62	##	0.05%	1.143	0.004	2.113	0.005	17.85	0.04	15.64	0.06	37.66	0.10
6	5-101221501	##	9361	169221	145466	348180	35	##	0.02%	1.143	0.003	2.117	0.006	17.86	0.03	15.64	0.04	37.75	0.07
7	5-101221701	##	15000	271236	232187	555445	79	##	0.02%	1.146	0.003	2.110	0.005	17.89	0.05	15.62	0.05	37.67	0.09
8	5-101221801	##	12373	223890	193952	463446	46	##	0.02%	1.148	0.004	2.106	0.004	17.88	0.02	15.58	0.04	37.60	0.05
9	5-101230401	##	7015	126613	109739	262641	35	##	0.03%	1.147	0.003	2.111	0.007	17.85	0.05	15.56	0.06	37.63	0.14
10	5-101230501	##	8880	160359	138927	333480	42	##	0.03%	1.147	0.004	2.116	0.005	17.85	0.04	15.55	0.06	37.72	0.11
11	5-101230601	##	14329	259464	224541	538054	37	##	0.02%	1.149	0.003	2.110	0.003	17.87	0.04	15.56	0.04	37.65	0.08
12	5-101230701	##	11732	212641	183439	439248	30	##	0.02%	1.144	0.003	2.116	0.005	17.88	0.06	15.64	0.06	37.79	0.10
13	5-101230901	##	14139	256818	221596	529791	32	##	0.01%	1.144	0.003	2.112	0.004	17.92	0.03	15.66	0.04	37.79	0.10
14	5-101231001	##	17147	310782	269426	643135	40	##	0.01%	1.144	0.003	2.110	0.004	17.88	0.04	15.63	0.04	37.68	0.07
15	5-101231101	##	15047	272315	235789	565032	50	##	0.02%	1.148	0.003	2.111	0.005	17.87	0.03	15.56	0.03	37.67	0.05
16	5-101231201	##	16318	296342	255758	612324	41	##	0.01%	1.145	0.003	2.115	0.005	17.92	0.04	15.66	0.04	37.83	0.06
17	5-101231301	##	15965	289932	250519	599442	37	##	0.01%	1.147	0.003	2.109	0.005	17.91	0.04	15.61	0.04	37.73	0.06
18	5-101231401	##	15467	280632	242670	581666	34	##	0.01%	1.150	0.003	2.109	0.004	17.89	0.02	15.56	0.03	37.68	0.08
19	5-101231501	##	13973	253370	218448	522721	35	##	0.02%	1.144	0.004	2.115	0.005	17.89	0.03	15.64	0.05	37.76	0.07
20	5-101231601	##	11786	213544	184863	442265	32	##	0.02%	1.147	0.004	2.110	0.003	17.88	0.04	15.58	0.05	37.65	0.04
21	5-101231701	##	10118	183638	158824	380740	25	##	0.02%	1.149	0.003	2.110	0.004	17.91	0.04	15.58	0.05	37.73	0.07
22	5-101240101	93	6311	114521	98967	236816	24	##	0.03%	1.146	0.004	2.111	0.006	17.92	0.06	15.63	0.06	37.77	0.14
23	5-101240201	83	6533	118478	102282	244885	18	##	0.02%	1.145	0.003	2.114	0.006	17.90	0.04	15.64	0.04	37.79	0.07
24	5-101240301	##	11074	200814	173562	416679	21	##	0.02%	1.148	0.004	2.115	0.006	17.89	0.04	15.58	0.03	37.77	0.07
25	5-101240501	99	12674	229964	198819	476264	21	##	0.01%	1.145	0.003	2.115	0.004	17.89	0.04	15.62	0.04	37.78	0.09
min										1.143		2.106		17.850		15.554		37.598	
max										1.150		2.117		17.921		15.663		37.832	
weighted mean										1.1460	0.0008	#	2.11175	0.00095	17.8872	0.0070	15.61	0.02	37.72
MSWD										1.5		1.4		1.13		2.70		3.40	
n=										25		25		25		25		25	

Sample locality 05

1	5-101220805	##	5480	99245	85173	205489	58	##	0.05%	1.158	0.004	2.107	0.006	17.98	0.03	15.52	0.04	37.83	0.08
2	5-101221805	##	8476	154306	132293	318983	59	##	0.03%	1.160	0.003	2.103	0.004	18.04	0.02	15.56	0.04	37.89	0.07
3	5-101230105	##	5072	92529	79243	191143	48	##	0.05%	1.161	0.004	2.102	0.005	18.11	0.06	15.60	0.08	38.02	0.16
4	5-101230205	##	5118	93100	79953	192412	49	##	0.05%	1.158	0.004	2.103	0.005	18.06	0.04	15.60	0.06	37.91	0.10
5	5-101230405	##	5250	95501	82088	197944	40	##	0.05%	1.157	0.003	2.109	0.005	18.06	0.05	15.61	0.07	38.02	0.13
6	5-101230505	##	6582	119705	102690	247831	59	##	0.04%	1.159	0.004	2.107	0.005	18.05	0.06	15.57	0.06	37.96	0.14
7	5-101230605	##	7310	132790	114404	275347	37	##	0.03%	1.154	0.003	2.110	0.004	17.97	0.05	15.57	0.06	37.85	0.07
8	5-101230705	##	7432	135695	116492	280615	72	##	0.03%	1.158	0.004	2.104	0.004	18.06	0.05	15.59	0.05	37.95	0.11
min										1.154		2.102		17.966		15.523		37.831	
max										1.161		2.110		18.114		15.609		38.021	
weighted mean										1.1580	0.0013	#	2.10560	0.00170	18.0310	0.0330	15.57	0.02	37.90
MSWD										1.5		1.6		3.9		1.3		1.8	
n=										8		8		8		8		8	

Sample locality 12

1	5-101230112	98	1409	25792	21884	52889	23	##	0.13%	1.172	0.005	2.086	0.008	18.32	0.18	15.63	0.13	38.15	0.31
2	5-101230412	##	1002	18379	15406	37398	27	##	0.20%	1.187	0.006	2.070	0.012	18.57	0.16	15.65	0.11	38.39	0.32
3	5-101230512	##	1590	29001	24624	59518	30	##	0.13%	1.171	0.007	2.088	0.008	18.30	0.12	15.62	0.10	38.15	0.21
4	5-101230612	##	1103	20168	16865	41101	35	##	0.21%	1.189	0.009	2.073	0.007	18.66	0.11	15.69	0.16	38.63	0.23
5	5-101231112	##	1928	35372	29997	72434	37	##	0.11%	1.172	0.005	2.083	0.008	18.38	0.08	15.67	0.06	38.23	0.16
6	5-101231212	##	2494	45661	38722	93433	39	##	0.09%	1.172	0.005	2.082	0.004	18.30	0.08	15.61	0.05	38.05	0.14
7	5-101231312	##	2885	53103	44806	108354	35	##	0.08%	1.178	0.004	2.076	0.007	18.37	0.07	15.59	0.07	38.07	0.16
8	5-101231412	##	1876	34705	28968	70336	42	##	0.13%	1.191	0.004	2.062	0.009	18.61	0.10	15.62	0.09	38.31	0.17
9	5-101231512	##	3137	57776	48861	118077	33	##	0.07%	1.176	0.004	2.079	0.007	18.34	0.06	15.59	0.07	38.07	0.14
10	5-101231612	##	1783	32714	27692	66982	29	##	0.11%	1.175	0.005	2.083	0.010	18.34	0.09	15.61	0.05	38.15	0.27
11	5-1012317012	92	1966	36193	30758	74227	22	##	0.09%	1.170	0.005	2.087	0.007	18.32	0.05	15.66	0.07	38.17	0.13
min										1.170		2.062		18.300		15.585		38.048	
max										1.191		2.088		18.660		15.688		38.626	
weighted mean										1.1778	0.0052	#	2.08010	0.00460	18.3760	0.0710	15.63	0.02	38.18
MSWD										9.0		3.8		6.4		0.8		2.7	
n=										11		11		11		11		11	

Sample locality 06

1	5-101220506	##	2389	42880	36951	88697	50	##	0.10%	1.154	0.005	2.105	0.008	17.98	0.09	15.58	0.10	37.79	0.20
2	5-101230106	##	3947	71482	61586	147866	40	##	0.06%	1.154	0.004	2.105	0.006	18.01	0.05	15.61	0.04	37.85	0.08
3	5-101230206	##	3349	60678	52292	125620	33	##	0.07%	1.154	0.004	2.106	0.006	18.02	0.06	15.62	0.08	37.91	0.18
4	5-101230406	##	2570	46106	39760	95425	46	##	0.09%	1.153	0.005	2.106	0.007	17.92	0.09	15.55	0.09	37.69	0.19
5	5-101230506	##	2264	40645	35069	84071	34	##	0.10%	1.152	0.004	2.104	0.005	17.95	0.07	15.58	0.08	37.73	0.16
6	5-101230606	##	1908	34194	29537	70880	33	##	0.12%	1.151	0.005	2.109	0.010	17.96	0.06	15.61	0.06	37.83	0.17
7	5-101230706	95	1297	23257	20049	48161	23	##	0.13%	1.153	0.004	2.107	0.011	17.96	0.09	15.57	0.07	37.79	0.16
8	5-101230806	73	1904	34444	29692	71277	15	##	0.08%	1.153	0.006	2.105	0.007	17.97	0.07	15.58	0.08	37.77	0.15
9	5-101231006	67	1551	28065	24196	58021	15	##	0.09%	1.153	0.004	2.103	0.010	17.99	0.11	15.60	0.11	37.79	0.27
10	5-101231106	82	1740	31494	27198	65157	17	##	0.09%	1.151	0.005	2.105	0.006	18.02	0.09	15.65	0.09	37.87	0.20
11	5-101231206	##	2929	53089	45750	109988	21	##	0.06%	1.154	0.004	2.108	0.004	17.98	0.08	15.59	0.07	37.86	0.18
12	5-101231306	##	4781	86855	74850	179858	23	##	0.04%	1.154	0.005	2.107	0.008	17.98	0.06	15.58	0.07	37.82	0.17
13	5-101231406	##	4645	84224	72737	174559	28	##	0.04%	1.151	0.003	2.109	0.005	17.95	0.07	15.59	0.06	37.80	0.15
14	5-101231506	##	5003	90736	78156	187389	26	##	0.04%	1.154	0.003	2.101	0.005	17.95	0.05	15.55	0.06	37.66	0.11
15	5-101231606	##	5405	98280	84738	203045	26	##	0.04%	1.153	0.004	2.102	0.005	17.98	0.04	15.59	0.05	37.75	0.09
16	5-101231706	96	4070	73687	63745	152749	17	##	0.04%	1.149	0.004	2.109	0.005	17.92	0.07	15.59	0.07	37.73	0.12
17	5-101240106	80	2704	49098	42349	101688	17	##	0.06%	1.153	0.005	2.107	0.006	18.00	0.05	15.61	0.05	37.87	0.12
18	5-101240206	75	2792	50688	43674	104760	17	##	0.05%	1.154	0.004	2.103	0.008	17.98	0.09	15.58	0.08	37.76	0.15
19	5-101240306	78	2580	46841	40438	97038	18	##	0.06%	1.152	0.004	2.108	0.006	18.00	0.06	15.63	0.08	37.88	0.13
20	5-101240406	60	2045	37009	31953	76517	15	##	0.07%	1.151	0.007	2.104	0.010	17.94	0.07	15.58	0.08	37.68	0.17
21	5-101240506	62	2467	44871	38702	92941	15	##	0.06%	1.153	0.004	2.107	0.006	18.01	0.07	15.62	0.06	37.90	0.10
min										1.149		2.101		17.916		15.545		37.664	
max										1.154		2.109		18.023		15.650		37.909	
weighted mean										1.1527	0.0009	#	2.10690	0.00140	17.9790	0.0140	15.60	0.02	37.80
MSWD										0.4		0.6		0.9		0.4		1.3	
n=										21		21		21		21		21	

Blank analyses over the whole analytical session

1	Blank	4	8	117	106	244
2	Blank	5	10	166	150	366
3	Blank	5	9	147	132	311
4	Blank	3	9	128	115	277
5	Blank	5	7	94	86	195
6	Blank	5	7	100	88	209
7	Blank	4	11	186	160	378
8	Blank	8	11	166	141	333
9	Blank	6	12	191	165	393
10	Blank	6	10	135	119	283
11	Blank	5	11	174	155	370
12	Blank	6	10	159	145	347
13	Blank	4	11	183	164	387
14	Blank	4	13	213	196	450
15	Blank	5	10	166	150	361
16	Blank	6	9	125	114	275
17	Blank	4	12	196	183	432
18	Blank	5	9	134	120	293
19	Blank	5	12	191	174	386
20	Blank	4	7	97	86	206
21	Blank	5	9	136	115	272
22	Blank	4	11	163	147	343
23	Blank	5	11	171	155	353

Supplementary information - Pb isotopic analysis

Pb isotopic analysis for determination of origin of Pb in the environment

Pb isotope analyses were performed at the Microgeochemistry Laboratory at the University of Gothenburg using an Agilent 8800 ICP-MS/MS. The sample introduction system used was an ASX-500 autosampler (Agilent), a peristaltic pump, a concentric glass nebulizer (MicroMist) and a Scott double-pass quartz glass spray chamber. The AS-500 autosampler was placed in an ISO 5 clean room environment and was connected to the ICP-MS in the adjacent Microgeochemistry laboratory with a tubing length of approximately 1 m.

All sample preparations were performed in the ISO 5 clean room environment using Milli-Q water (resistivity > 18.2 MΩ cm) and ultrapure nitric acid (NORMATOM®, VWR chemicals). Samples, reference waters and blanks were prepared with a matrix of 2% HNO₃. A dilute solution of the digested common lead isotopic Standard Reference Material (SRM) 981 (NIST, Cantanzaro et al. 1968) was used as primary standard to correct for drift and mass bias. The approximate lead concentration of this primary reference solution was 11 µg/l. AQUA-1 natural drinking water certified reference material (NRC Canada, (Yeghicheyan et al., 2021)) was analysed as secondary reference solution to estimate accuracy and precision. Weighted averages for all lead isotope ratios for five interspersed AQUA-1 analyses overlap in 2 s with the Pb isotopes ratios reported by Yeghicheyan et al. 2021 and their expanded uncertainties. To ascertain identical lead ratios for lead isotopes measured across pulse counting mode, two other dilutions of NIST SRM 981 with concentrations of approximately 1.1 µg/l and 5.5 µg/l were run repeatedly throughout the measurement session. These lead concentrations are similar to the lead concentration of the water samples taken from Skogaryd. Pb isotopes. Additionally, a blank was measured after every standard and sample block and used to subtract the mercury and lead background. ²⁰⁴Hg on monitored counts per second (CPS) on mass 204 was subtracted by using CPS on ²⁰²Hg and the isotopic abundance for both isotopes (CIAAW, 2021)).

The operating conditions of the ICP-MS and acquisition parameters are listed in Table S2, S3 and S4. The ICP-MS was run in MS/MS mode with NO₂ as reaction gas. Tuning of the instrument was performed. The peak shape and position were optimised for masses 206, 207 and 208 for both quadrupoles using diluted NIST SRM 981 after auto-tune of the lenses using a 10 µg/l Li, Y, Ce, Tl, and Co Tuning solution (Agilent).

Uncertainties reported in the data table include the standard error of the 10 replicates added in quadrature with the excess scatter of the primary reference solution NIST SRM 981 of the respective ratios. The uncertainty in the ²⁰⁴Hg correction was propagated where necessary. All uncertainties are given at 2se. Systematic uncertainties are not reported in the data tables but include the ratio uncertainty of NIST SRM 981 and the long-term excess scatter.

Reference

Yeghicheyan, D., Grinberg, P., Alleman, L. Y., Belhadj, M., Causse, L., Chmeleff, J., Cordier, L., Djourae, I., Dumoulin, D., Dumont, J., Freydier, R., Mariot, H., Cloquet,

C., Kumkrong, P., Malet, B., Jeandel, C., Marquet, A., Riotte, J., Tharaud, M., ... Mester, Z. (2021). Collaborative determination of trace element mass fractions and isotope ratios in AQUA-1 drinking water certified reference material. *Analytical and Bioanalytical Chemistry*, 413(20), 4959–4978. <https://doi.org/10.1007/s00216-021-03456-8>