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Supporting information

on the article

Groundwater uranium origin and fate control in a river valley aquifer

by

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- 12 pages, 5 figures, 7 tables -

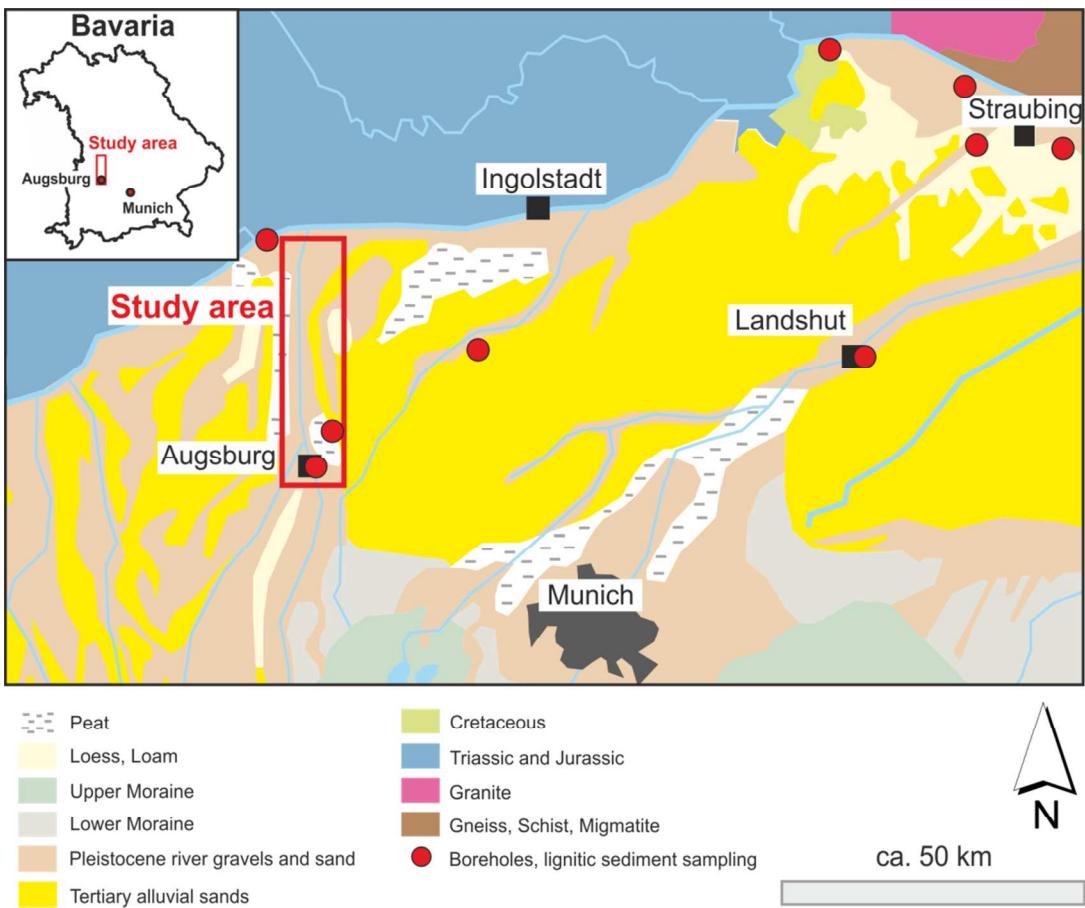


Figure S1. Location of the study area in Bavaria (upper left), geological overview map of the study area and its surroundings, and location of the 9 boreholes sampled for lignitic layers from the core warehouse of the Bavarian Environment Agency.

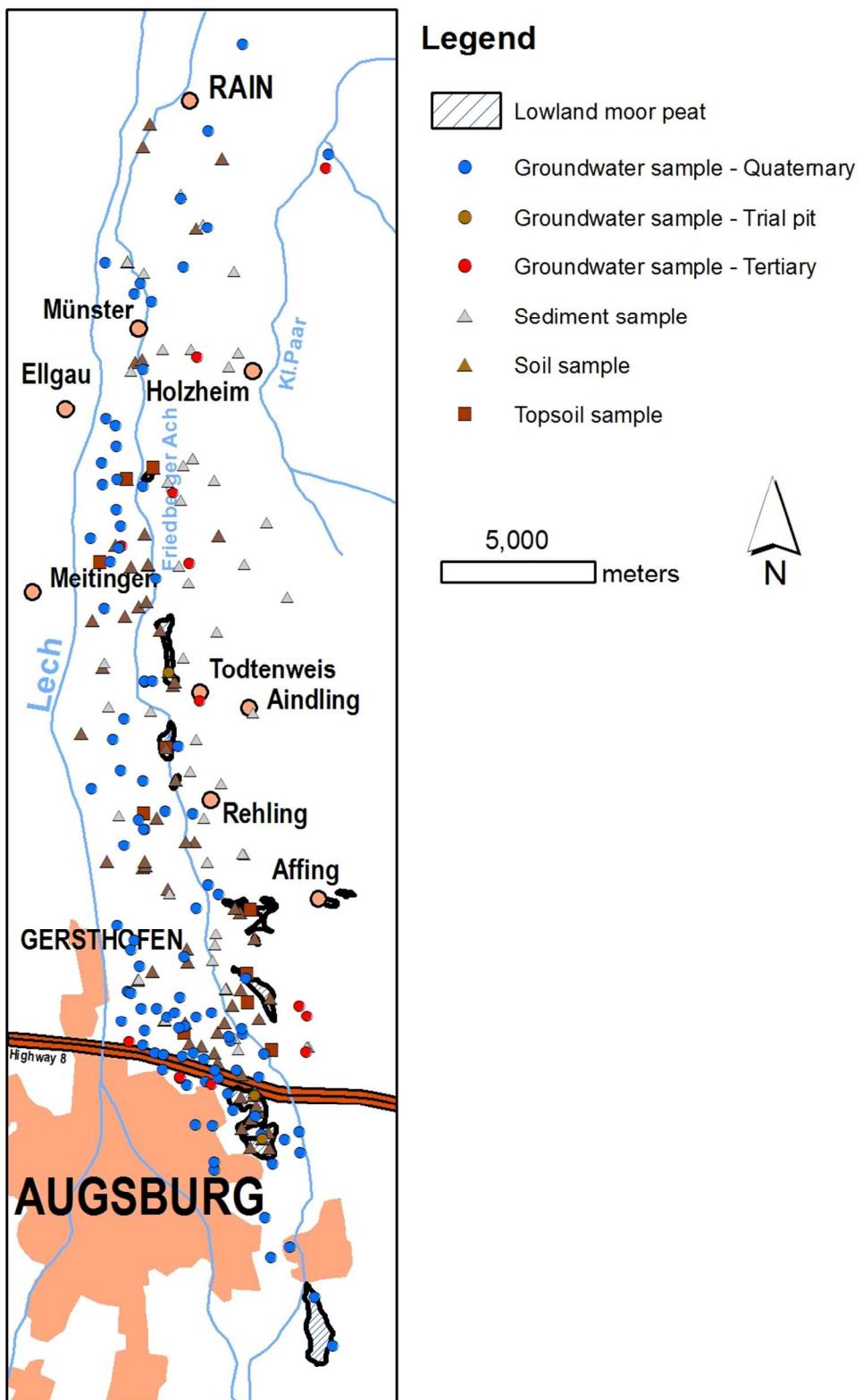


Figure S2. Study area map and sampling locations.

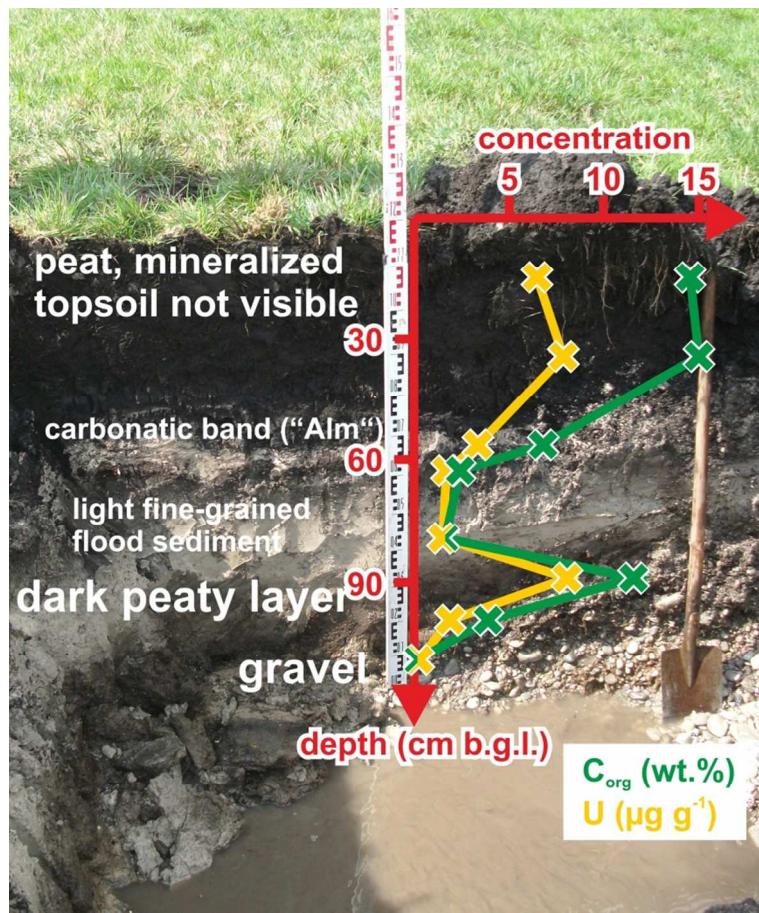


Figure S3. Profile and U/C_{org} development in trial pit 2.

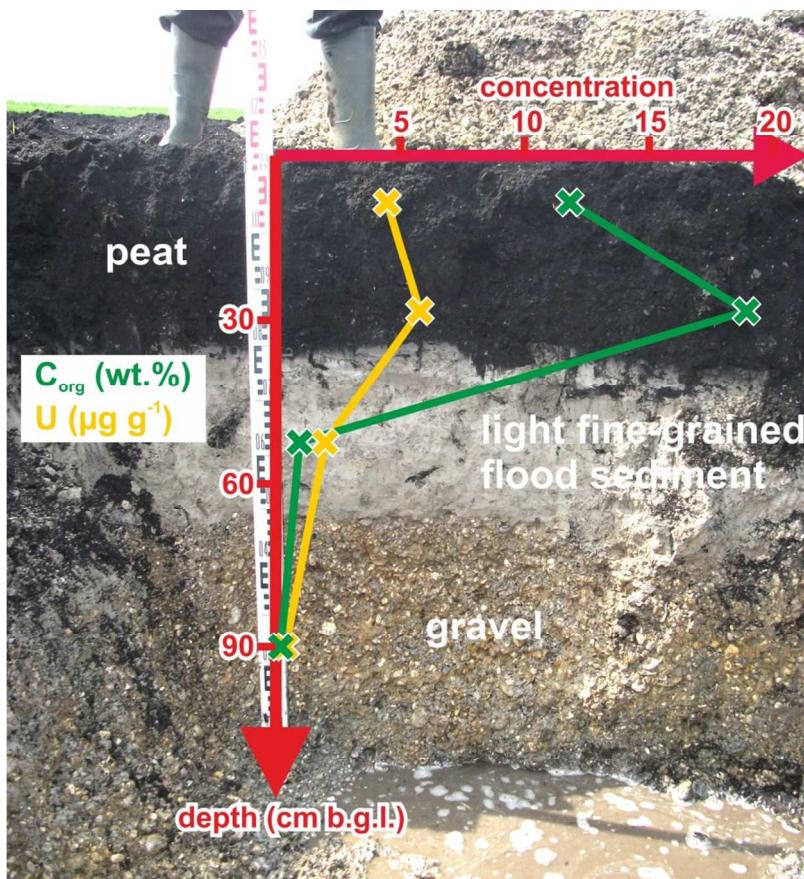


Figure S4. Profile and U/C_{org} development in trial pit 3.

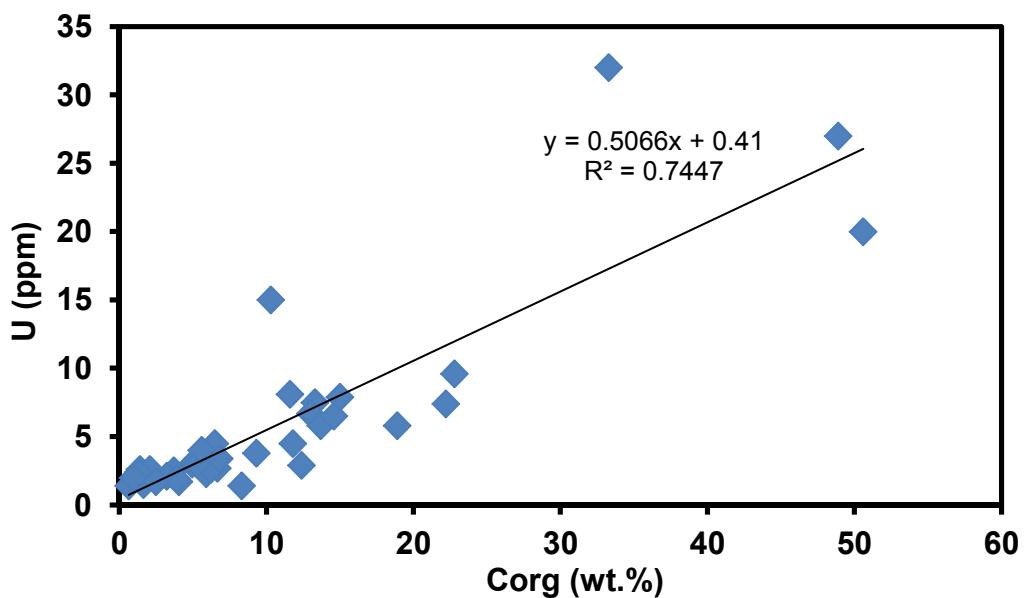


Figure S5. Scatter plot and regression of U and C_{org} in soil samples.

Table S3. Soil geochemical data (trial pit samples).

Sample groups and sample no.	pH	organic C	inorganic C	N	S	As	Co	Cr	Cu	Ni	Pb	Sb	U	V	Zn
		wt.%	wt.%	wt.%	wt.%	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
trial pit 1															
cf. Paper Fig. 2															
77	7.5	0.65	4.03	0.05	0.11	5.4	<2.1	9.1	<10	8	<10	<0.14	1.4	9.1	<21
78	7.5	1.40	6.21	0.05	0.17	5.3	<2.1	11	<10	8.7	<10	<0.14	2.6	13	<21
79	7.4	5.61	3.27	0.39	0.17	9.5	4.3	30	17	24	<10	0.20	4.0	38	37
80	6.8	33.3	0.37	1.75	0.70	100	7.3	22	19	43	<10	0.24	32	28	35
81	7.0	48.9	0.91	2.91	1.16	170	<2.1	<5.5	<11	13	<10	<0.14	27	5.6	<21
82	7.1	50.6	1.55	3.90	0.80	63	<2.1	9.6	15	10	<10	<0.14	20	9.8	<21
83	7.4	12.4	6.83	1.16	0.22	39	<2.1	17	12	5.7	18	0.26	2.9	43	38
84 ("Alm")	7.6	3.80	11.2	0.27	0.05	46	<2.1	<5.5	<10	4.1	<10	<0.14	2.0	<4.1	<21
85 (Fe hydr.)	7.5	17.3	3.85	1.34	0.29	80	6.7	<5.5	<10	14	11	<0.14	23	5.4	51
86 (plant fibre)	7.1	21.5	0.53	1.20	0.43	69	7.1	34	22	33	<10	0.29	20	40	51
trial pit 2															
cf. Fig. S3															
87	7.5	2.07	5.76	0.11	0.20	7.7	<2.1	11	<10	8	<10	<0.14	2.6	10	<21
88	7.7	3.90	10.7	0.24	0.23	13	<2.1	<5.5	<10	5.1	<10	<0.14	1.9	5.5	<21
89	7.5	11.6	7.47	0.65	1.10	41	3.5	14	16	17	<11	<0.14	8.1	16	26
90	7.8	1.63	9.17	0.05	0.05	8.5	2.5	16	10	14	<10	<0.14	1.5	20	<21
91	7.7	2.48	8.82	0.17	0.05	8.1	3.0	18	13	16	<10	<0.14	1.7	23	23
92	7.5	6.79	9.31	0.48	0.16	20	3.0	12	28	21	<10	0.26	3.4	19	<21
93	7.5	15.0	0.68	1.25	0.35	44	14	70	64	64	17	0.56	7.9	94	72
94	7.4	14.6	2.86	1.30	0.27	110	8.6	29	28	29	23	1.30	6.5	48	57
trial pit 3															
cf. Fig. S4															
95	7.5	1.29	4.17	0.05	0.19	3.6	2.2	10	<10	8.9	<10	0.23	2.4	12	<21
96	7.8	0.95	7.57	0.05	0.05	1.0	2.2	11	<10	8.7	<10	0.15	2.0	16	<21
97	7.2	18.9	1.84	1.52	0.31	14	6.4	38	27	24	24	0.72	5.8	65	58
98	7.0	11.8	0.93	1.04	0.18	14	8.4	54	30	33	26	0.68	4.5	83	71

Table S4. Mineralogical composition of sediments and soils (XRD-Rietveld data).

The software BGMIN was used to perform quantitative phase analysis which consists of an automatic, whole powder-pattern calculation and refinement of structural data (provided as mineral structure files of ideal phases ranging in unit cell axial lengths, developed by the Institute of Clay and Interface Mineralogy, RWTH Aachen University) against observed data. The programme performs an automated background refinement, allowing for the separation of an intensity difference curve containing the diagnostic Bragg reflections. These were allocated to mineral phases with the help of the aforementioned structure files and the database MINCRYST. Single phase structural information and sample mineralogical composition were refined aiming for minimum deviation, i.e. best fit, between model and observed data.

	Sample groups and sample no.	Mineralogical composition (wt.%)
Sediments	Fe-rich concretions in Tertiary sands	
	12	Qz: 55.7; Ms: 31.3; Fsp: 6.7; Cm: 5.2; Gt: 1.1
	13	Qz: 79.3; Fsp: 8.1; Cm: 4.6; Ms: 4.3; Ttn: 2.3; Gt: 1.4
	15	Qz: 54.9; Alm: 29.9; Fsp: 3.8; Ms: 3.7; Cm: 3.6; Ttn: 2.3; Gt: 1.6
	Cley lense in Tertiary sands	
	16	Qz: 35.0; Cm: 24.2; Ms: 16.4; Ttn: 8.5; Fsp: 7.4; Anh: 6.5
	Pure Tertiary sands	
	17	Qz: 82.5; Ms: 11.2; Fsp: 4.7
	Loesses and loess loams	
	29	Qz: 69.0; Ms: 13.5; Fsp: 9.1; Cm: 6.8
	30	Qz: 39.2; Dol: 26.7; Cal: 18.6; Fsp: 8.5; Ms: 5.2; Cm: 1.7
	Alluvial valley deposits	
	44	Qz: 56.4; Dol: 13.7; Ms: 8.8; Cal: 7.3; Cm: 6.9; Fsp: 6.6
Soils	Calcaric-humic gleysol	
	28	Cal: 88.0; Dol: 6.3; Qz: 5.7
	Gley	
	40	Qz: 35.3; Dol: 32.3; Cal: 13.5; Ms: 8.6; Fsp: 5.5; Cm: 4.4
	Calcaric fluvisol	
	49	Dol: 53.2; Cal: 17.7; Qz: 16.6; Ms: 5.9; Fsp: 4.0; Cm: 2.6
	Calcaric arenosol	
	57	Qz: 42.1; Dol: 25.4; Cal: 15.1; Ms: 8.9; Fsp: 4.5; Cm: 3.8
Trial pit 1		
	84 ("Alm")	Cal: 99.4
Trial pit 2		
	90	Cal: 59.0; Dol: 29.6; Qz: 9.7; Fsp: 1.7
Trial pit 3		
	96	Dol: 60.9; Qz: 26.5; Cal: 9.1; Fsp: 3.5

Table S5. LA-ICP-MS data for sediments and soils.

	Si LOD	Al 1.4	Ca 5000	Fe 95	Mn 7.1	As 33	Cr 48	Ni 8.0	Pb 0.9	Th 0.2	U 0.2	V 6.0	Zn 39
Sample group and point analysis no.	wt.%	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
Lignitic sediment													
5-1	81.5	98025	8130	104243	597	1302	350	203	402	22.2	299	384	351
5-2	54.9	106642	7370	87791	336	822	264	139	104	21.2	219	348	260
5-3	62.9	128006	5185	86898	441	626	269	139	298	16.8	138	313	329
5-4	96.3	120214	16264	138320	706	3557	286	146	599	23.7	243	602	439
10-1	5.1	8733	< 5000	68419	119	456	< 48	55	9.1	4.9	62.5	89	< 39
10-2	12.9	26245	200897	41184	256	319	71	41	10.5	5.4	40.5	94	76
10-3	11.3	15139	< 5000	105684	270	536	59	110	15.0	5.7	60.7	116	87
10-4	< 1.4	4124	< 5000	66441	105	521	< 48	45	2.8	4.6	61.6	97	< 39
10-5	< 1.4	4270	8114	27965	175	159	< 48	19	2.3	1.0	41.6	47	< 39
10-6	< 1.4	2760	20003	13847	165	178	< 48	15	0.9	0.6	25.6	32	< 39
Fe-rich concretion													
14-1	11.0	n.a.	9290	*	81	16376	6462	97	4.8	0.3	8.5	607	174
14-2	8.1	n.a.	8689	*	246	18721	878	91	4.7	0.3	9.6	439	185
14-3	10.1	n.a.	7547	*	451	15391	1313	119	6.2	0.6	9.8	505	259
14-4	11.0	n.a.	5901	*	171	11087	5283	60	2.6	0.3	6.9	1210	251
14-5	6.4	n.a.	< 5000	*	99	10888	91	39	6.4	1.1	5.2	384	93
14-6	44.2	n.a.	< 5000	*	91	2961	74	19	1.3	2.3	1.7	123	76
* too high for quantification with used standard													
Lowland moor peat													
80-1	41.9	26647	13528	9440	94	32	< 48	40	8.6	2.5	8.9	65	70
80-2	36.7	27139	12601	25315	249	428	< 48	32	10.8	3.0	4.3	85	69
80-3	25.1	42820	48996	22003	257	160	114	87	18.3	6.8	52.5	110	65
80-4	24.1	36565	49789	15127	198	100	692	148	21.2	4.9	53.0	92	147
80-5	32.9	55647	38828	14809	290	< 33	144	79	20.5	11.6	26.7	111	71
80-6	29.5	54244	53733	18974	221	144	109	84	16.3	6.2	51.3	135	85
97-1	18.2	12922	13614	5626	59	< 33	< 48	< 8	9.0	1.0	1.1	31	< 39
97-2	12.6	29599	42554	23790	276	47	62	37	26.7	4.6	7.3	110	66
97-3	20.0	49956	52138	23993	1284	< 33	90	47	38.2	6.2	9.8	150	74
97-4	18.1	40169	42444	19007	1533	< 33	83	38	33.7	6.6	7.1	130	65
97-5	23.3	47245	39555	29504	476	40	88	49	48.0	6.6	10.6	191	73
97-6	18.6	38610	58572	19260	1344	< 33	67	47	31.2	6.9	11.0	117	42

Table S7. Hydrochemistry data: Tertiary aquifer.

Sample no.	pH	temp °C	eC µS/cm	Eh mV	O2 mg/l	DOC mg/l	Ca mg/l	Mg mg/l	Na mg/l	K mg/l	HCO3 mg/L	Cl mg/l	SO4 mg/l	NO3 mg/l	Fe mg/l	As mg/l	Cu mg/l	Mn mg/l	Sr mg/l	V mg/l	Zn mg/l	U µg/l
101	7.3	10.9	501		0.2	0.5	71	29	5.9	0.9	348	1.0	14	<0.5	0.20	0.001	<0.001	0.049	0.64	<0.0001	<0.01	0.4
102	7.5	10.7	584		9.2	0.5	85	26	4.9	0.6	247	40	25	62	<0.01	<0.001	<0.001	0.20	0.0003	<0.01	3.7	
103	7.4	10.3	441		0.6	<0.5	73	20	3.0	0.6	314	2.0	20	2.2	0.04	0.002	<0.001	0.044	0.18	<0.0001	0.01	1.5
104	7.2	10.2	770		9.0	0.5	118	31	8.5	0.8	311	34	46	107	<0.01	0.001	<0.001	<0.001	0.14	0.0002	<0.01	1.8
105	7.5	11.0	604		1.0	0.7	87	28	4.3	1.1	287	16	62	0.05	1.10	0.0025	<0.001	0.050	0.47	<0.0001	<0.01	0.5
106	7.6	9.7	522		0.9	0.5	82	28	3.7	0.9	280	22	60	0.05	0.20	0.002	<0.001	0.006	0.14	<0.0001	<0.01	5.7
107	7.6	9.4	505		1.8	<0.5	78	29	3.6	0.8	319	5.8	34	7.4	<0.01	<0.001	<0.001	0.002	0.13	<0.0001	<0.01	3.0
108	7.1	8.9	772		1.5	0.7	128	36	6.4	1.1	386	48	73	15	0.10	<0.001	0.022	0.060	0.24	<0.0001	0.12	6.0
109	7.5	10.1	797		10.7	0.7	108	35	19.3	0.7	326	61	42	76	0.01	0.001	0.007	<0.001	0.14	0.0002	0.03	1.5
110	7.4	10.8	512		0.3	<0.5	82	28	2.9	1.1	409	1.5	4.4	<0.5	0.80	0.01	<0.001	0.070	0.56	<0.0001	<0.01	0.2
111	7.4	12.5	525	190	0.1	<0.5	80	31	3.1	0.9	394	1.5	2.8	<0.5	0.50	<0.001	<0.001	0.060	0.75	<0.0001	0.03	0.3
112	7.3					<0.5								<0.5							0.9	
113	7.6					<0.5								<0.5							0.4	
114	7.3					0.8								<0.5							1.3	