

Supporting Information

Multicomponent statistical analysis to identify flow and transport processes in a highly complex environment

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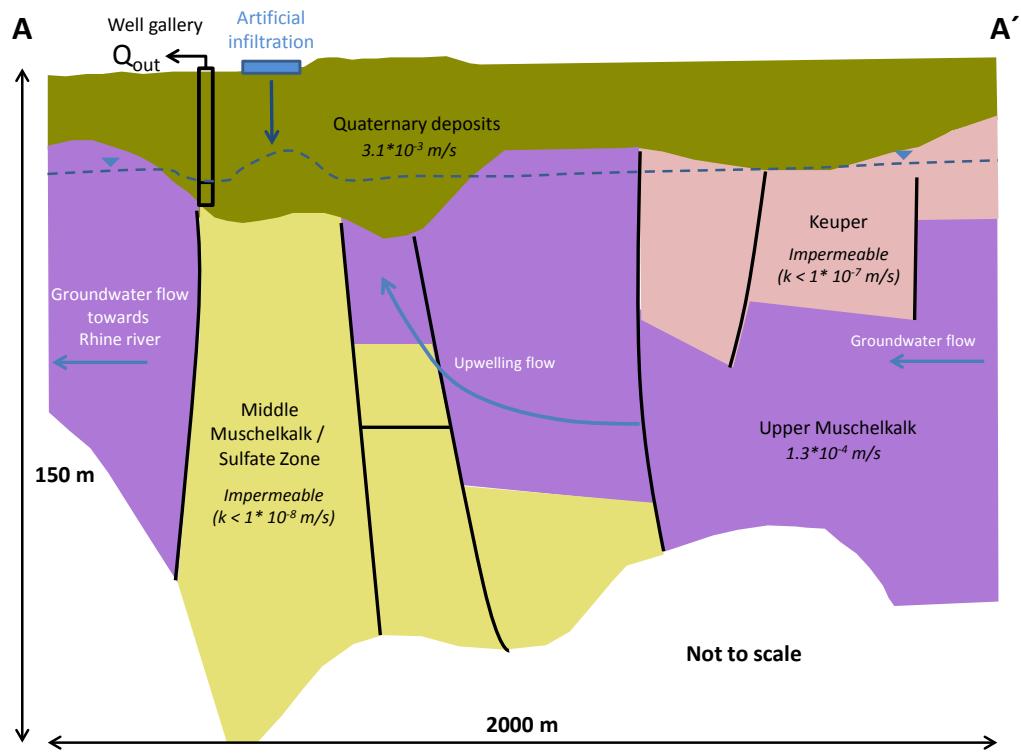


Figure S1: Schematic cross-section from south(A') to north (A) with the different geological units and expected flow directions.

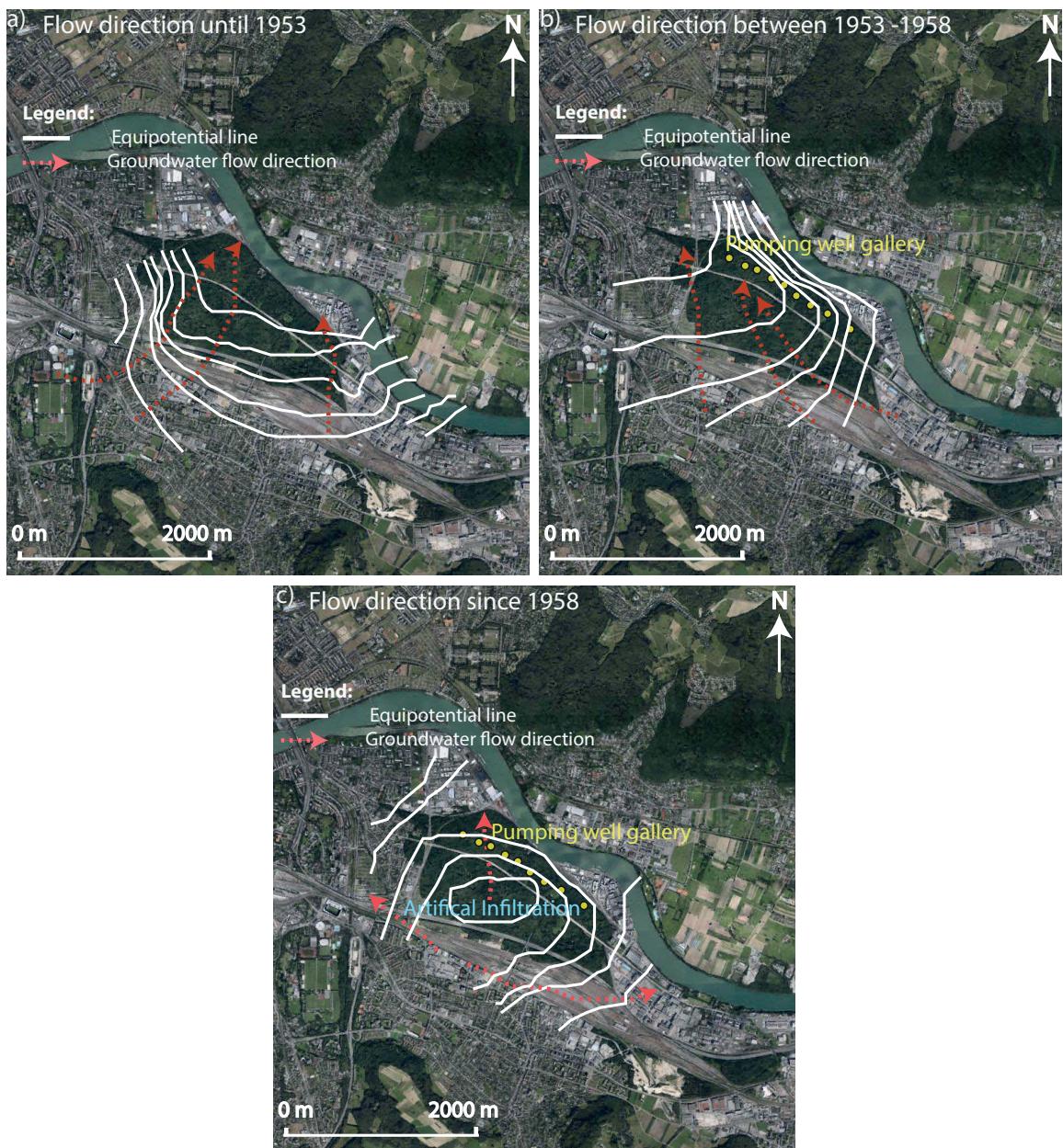


Figure S2: Schematic overview about the influence of the changing boundary conditions with landfill (orange), equipotential lines (white) and groundwater flow direction (red dashed line) a) Natural flow direction until 1953, b) Flow direction between 1953-1958 with location of the pumping well gallery (yellow) and c) Flow direction since 1958 with location of the pumping well gallery (yellow) and artificial infiltration (light blue). (Figure modified after Huggenberger et al., 2009 and Huggenberger and Epting (2011)).

Component: PCE

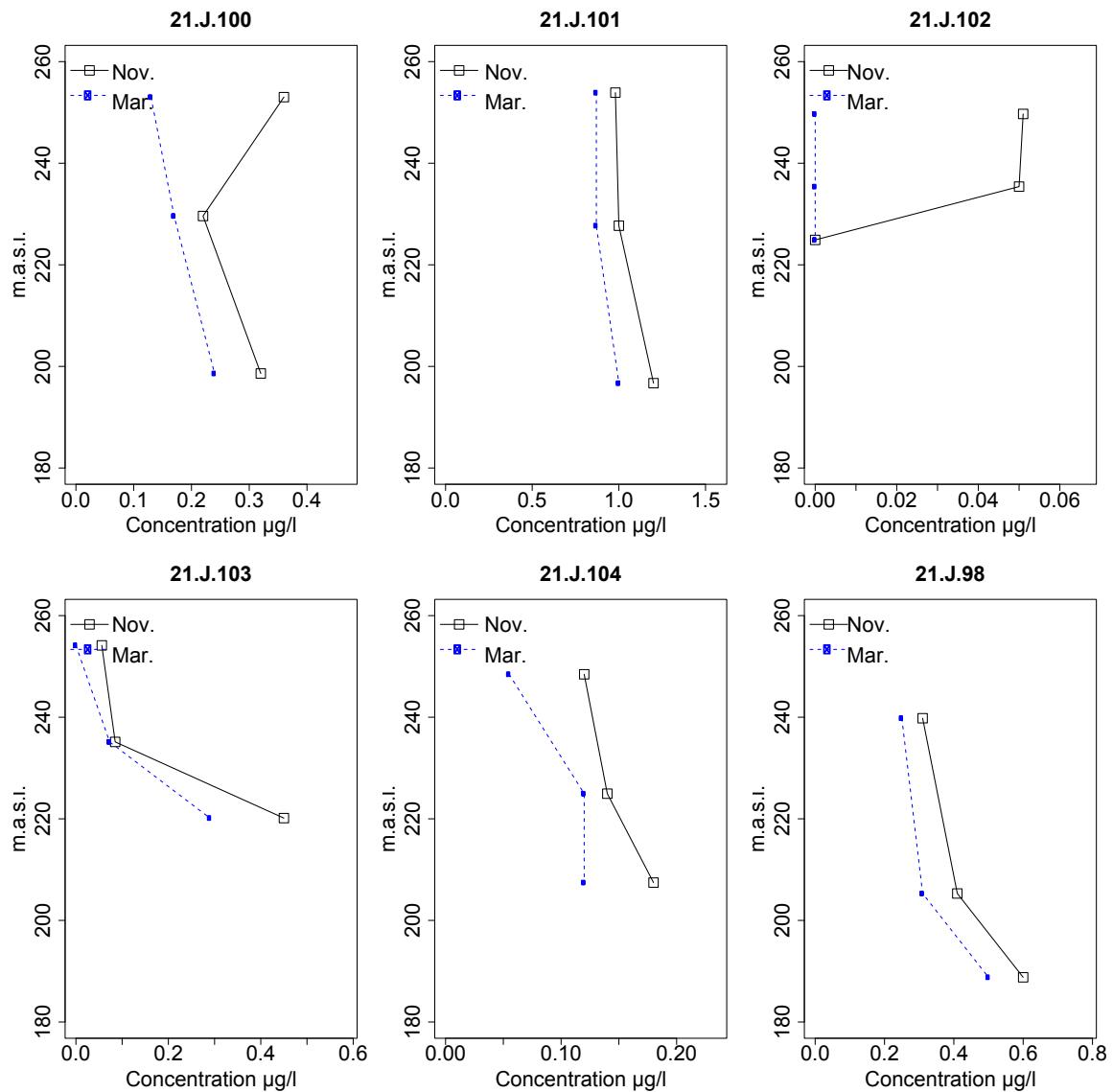


Figure S3: PCE concentrations at the multi-level wells for the two field campaigns in November 2014 and March 2015.

Component: TCE

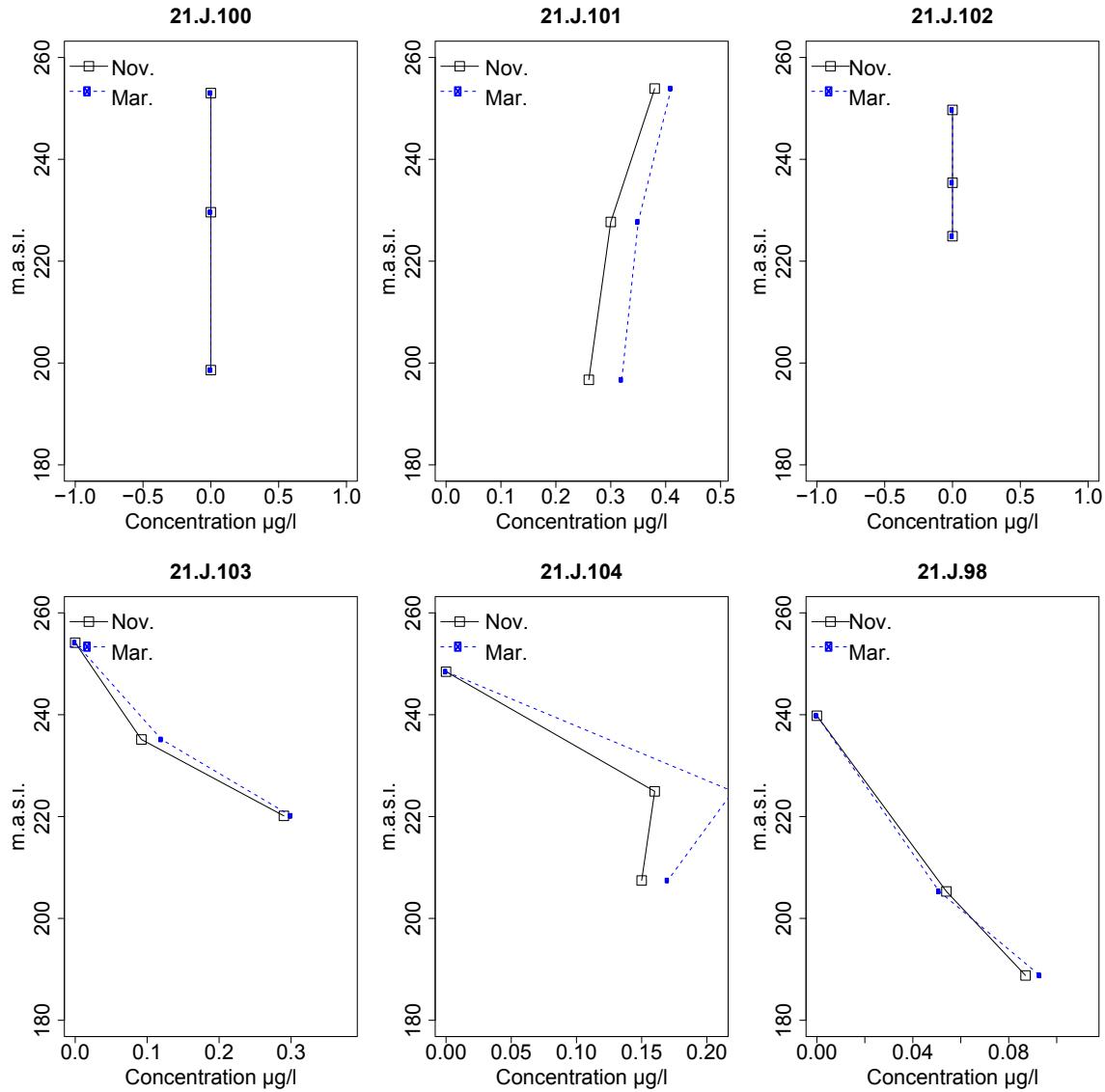


Figure S4: TCE concentrations at the multi-level wells for the two field campaigns in November 2014 and March 2015.

Component: HeCBD

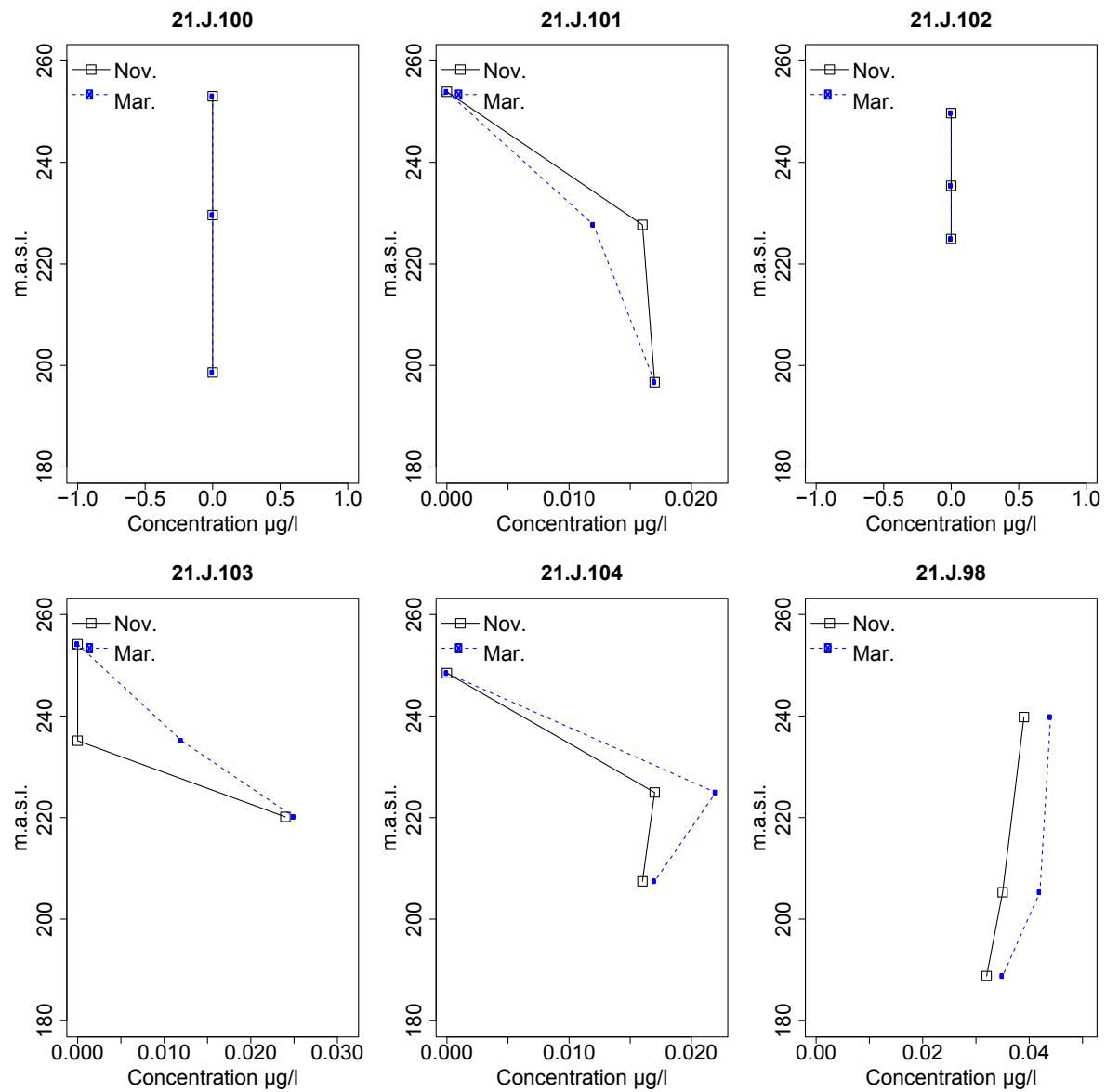


Figure S5: TeCBD concentrations at the multi-level wells for the two field campaigns in November 2014 and March 2015.

Component: TeCBD

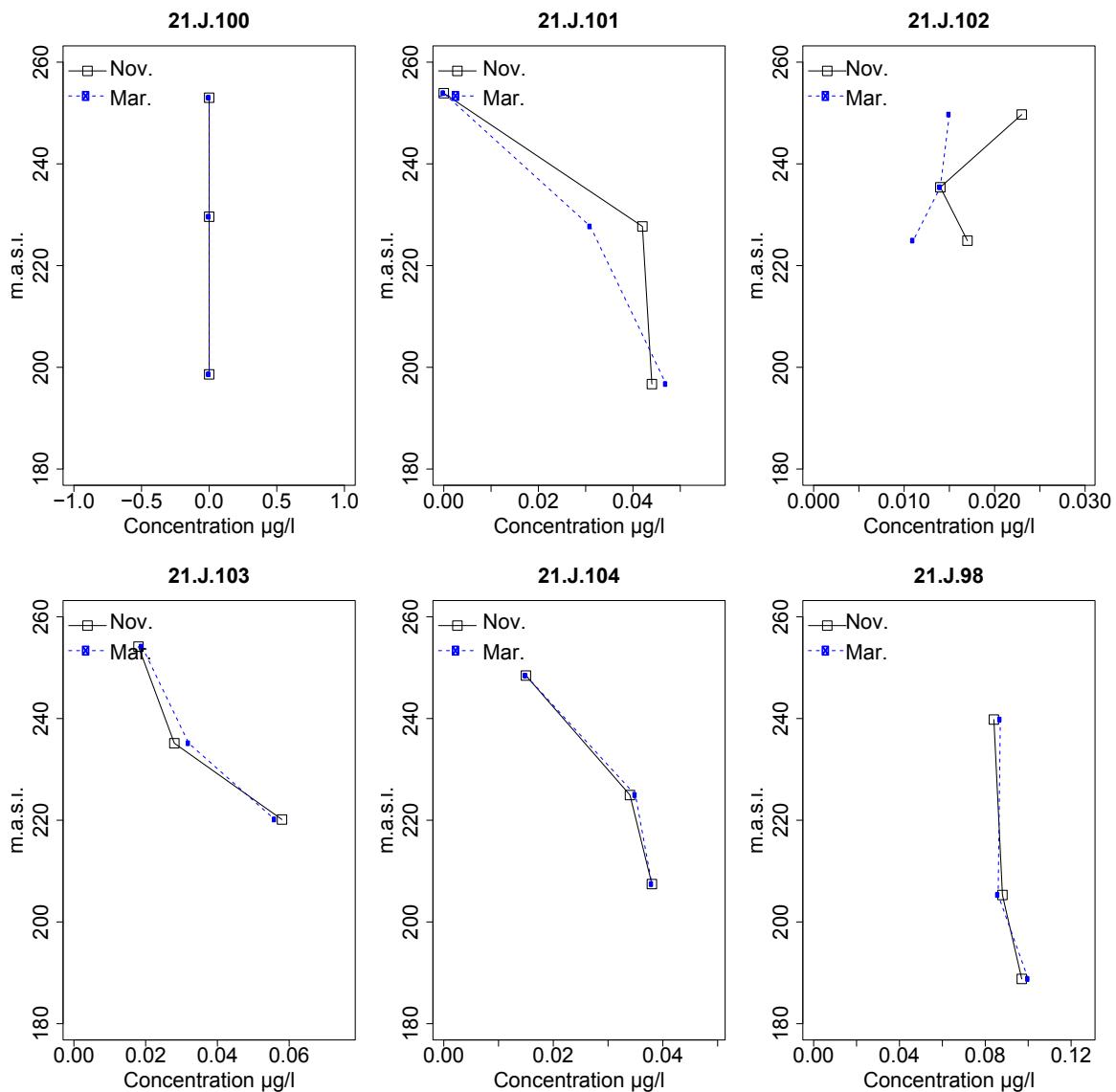


Figure S6: HeCBD concentrations at the multi-level wells for the two field campaigns in November 2014 and March 2015.

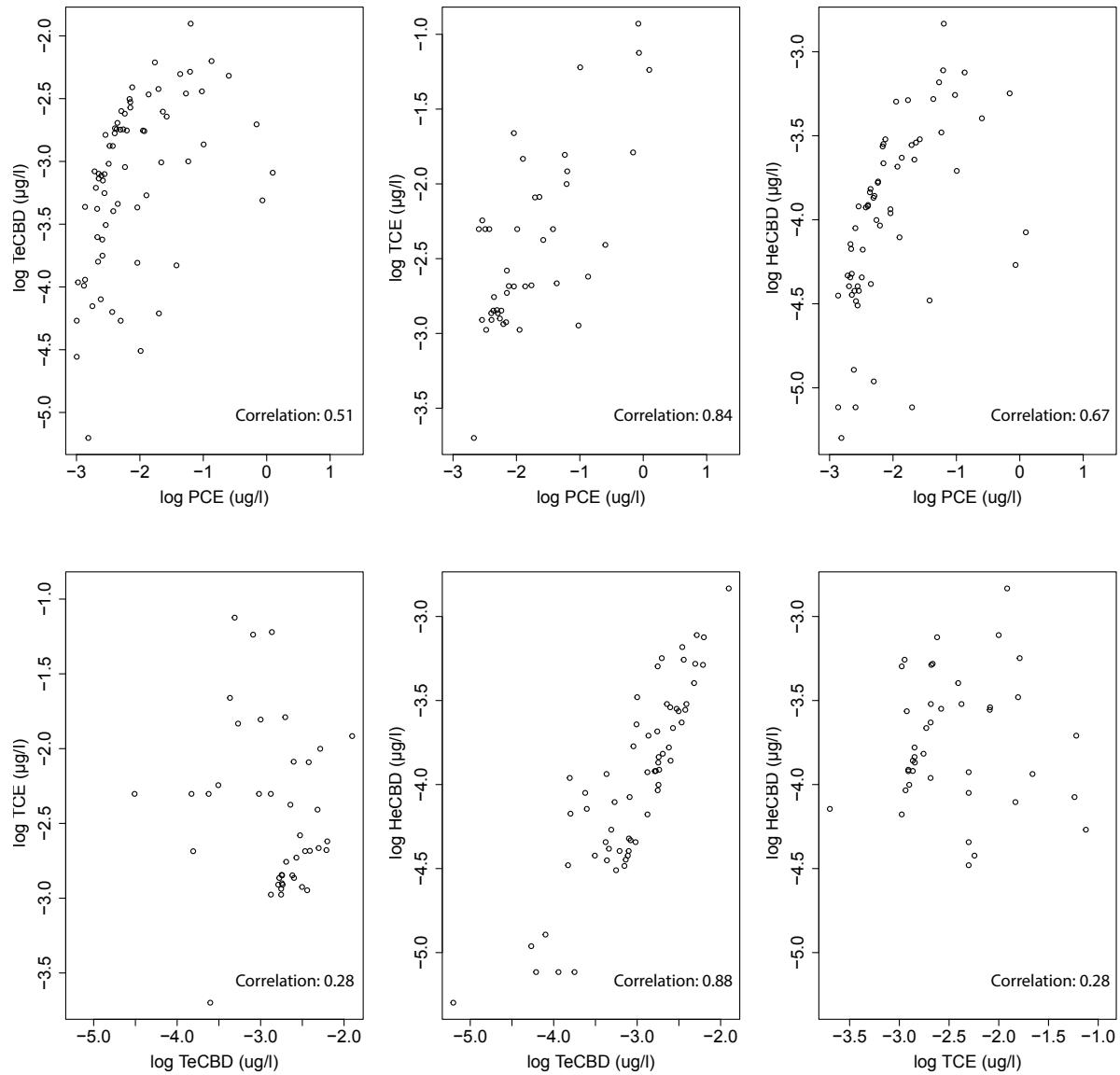


Figure S7: Plot between selected compounds with correlation coefficient (R^2). The different colours indicate the different cluster numbers. Note that the weak correlation (0.22) between TCE and TeCBD is probably due to a smaller data set for TCE. Only a few identical observations for both, TCE and TeCBD exist and limit therefore a comparison between these compounds.

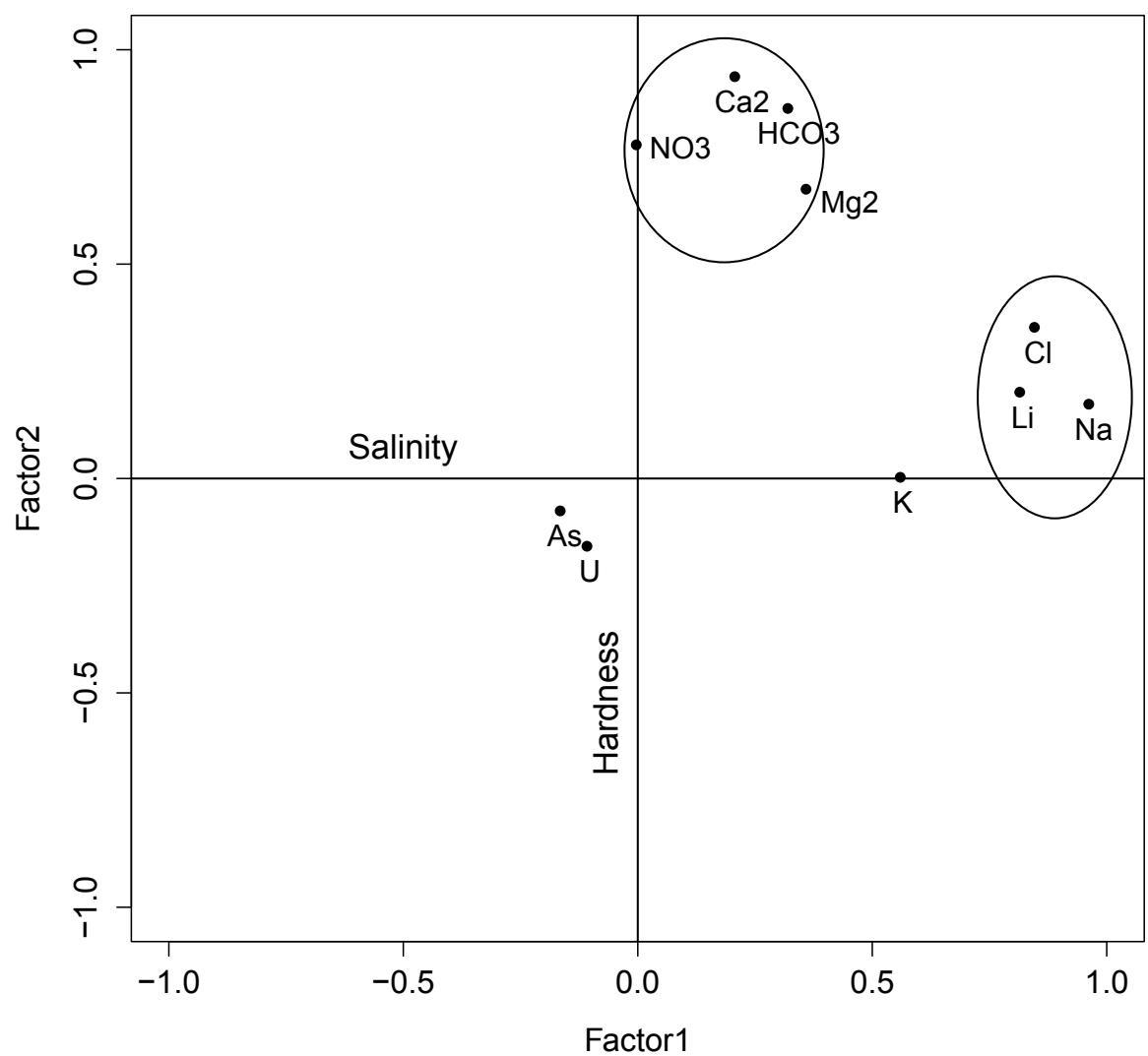


Figure S8: Factor analysis scores for factor 1 vs 2, whereas factor 1 indicates the salinity and factor 2 the hardness.

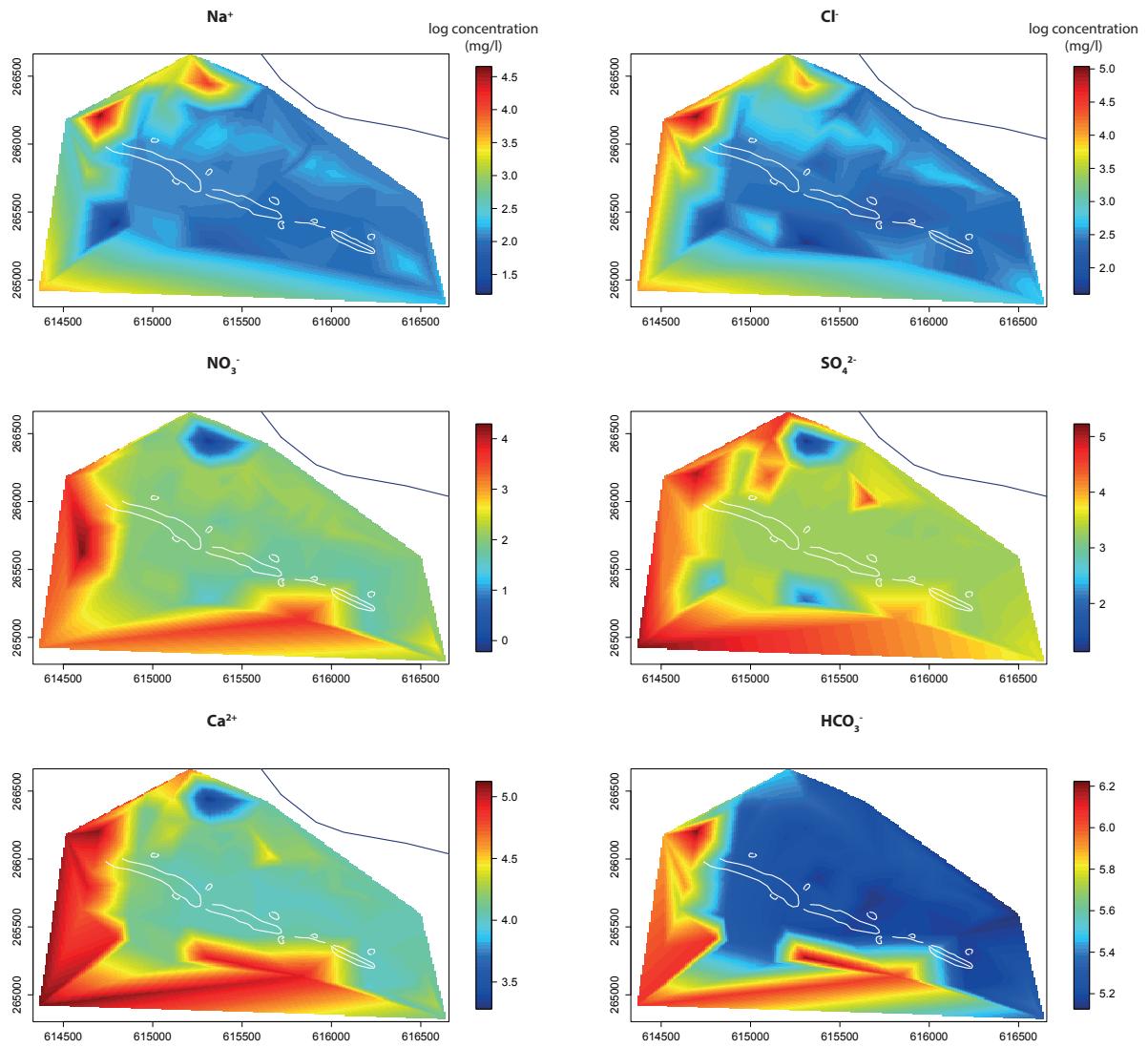


Figure S9: Spatial distribution of log concentration of Na^+ , Cl^- , NO_3^- , SO_4^{2-} , Ca^{2+} and HCO_3^- in the study area.

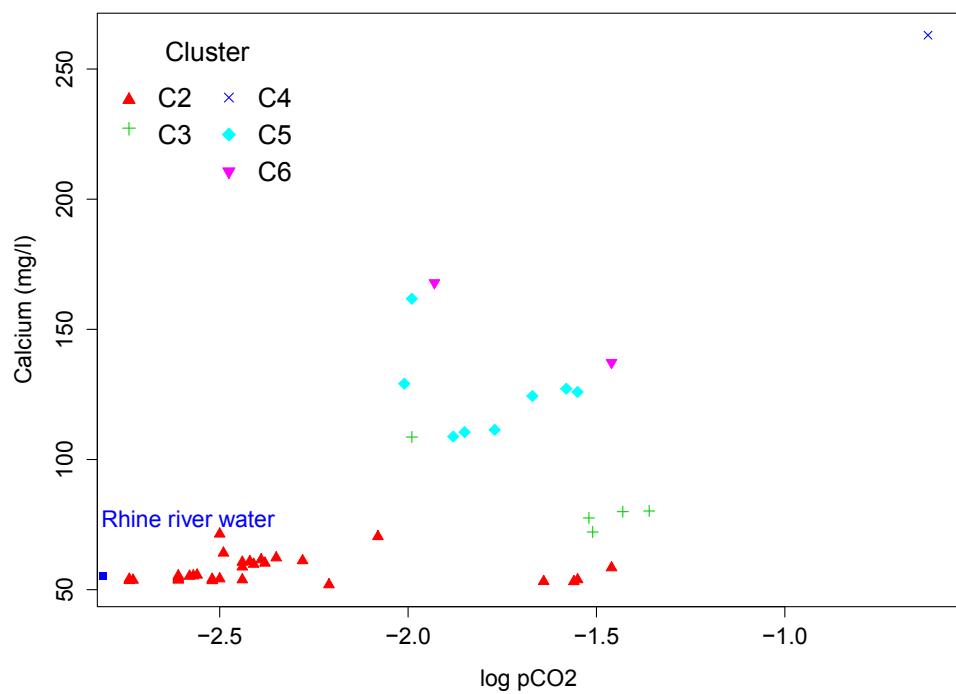


Figure S10: Calcium as a function of $p\text{CO}_2$. Sampling campaign in November 2014.

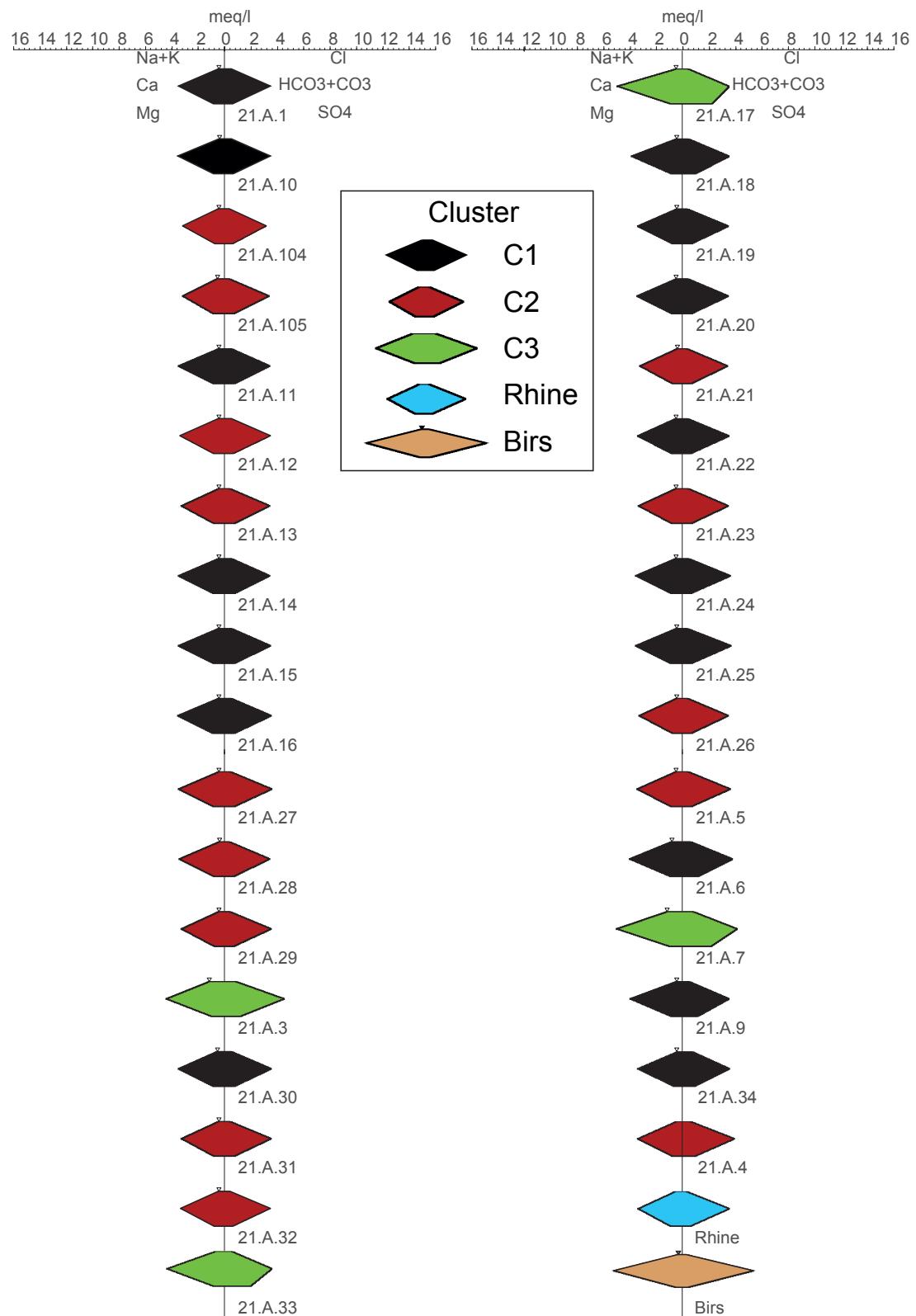


Figure S11: Stiff diagram of major ions concentrations as milli-equivalents per litre for all extraction wells. Different colours indicate the cluster number and the two river waters of Birs and Rhine.

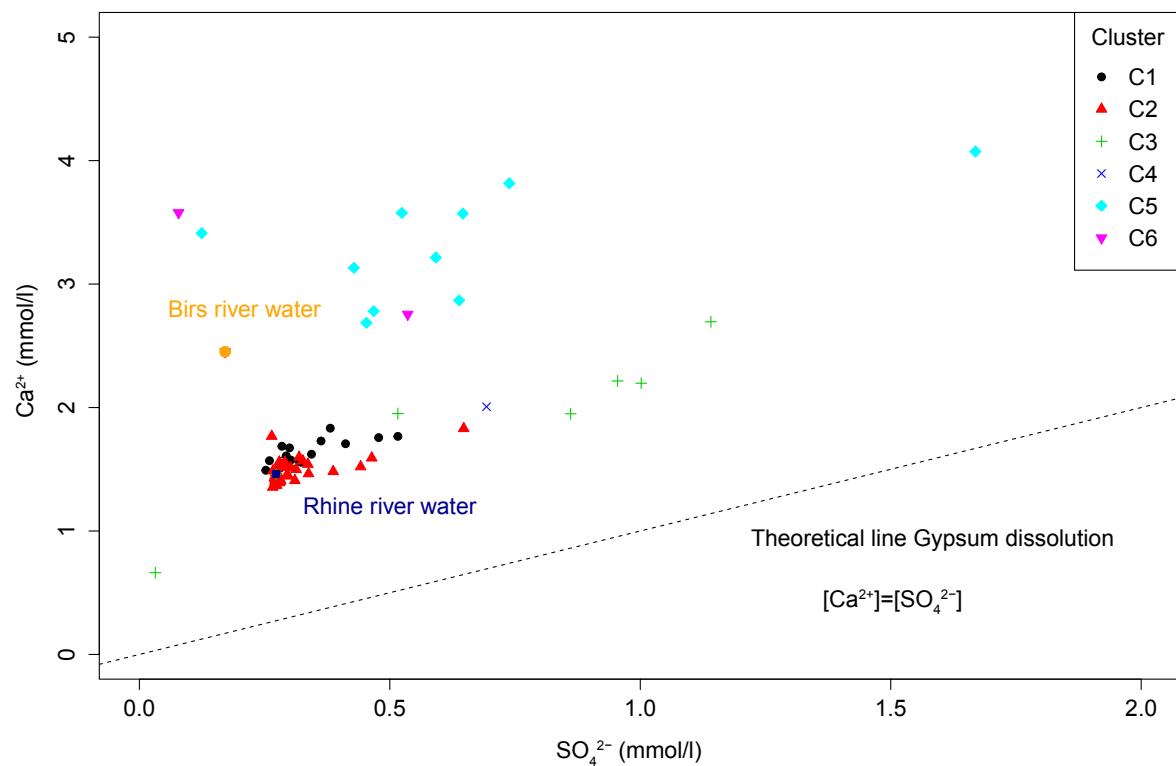


Figure S12: Plot of SO_4^{2-} and Ca^{2+} (mmol/l) for the analysed data compared with the theoretical 1:1 line. Different colours indicate the cluster groups.

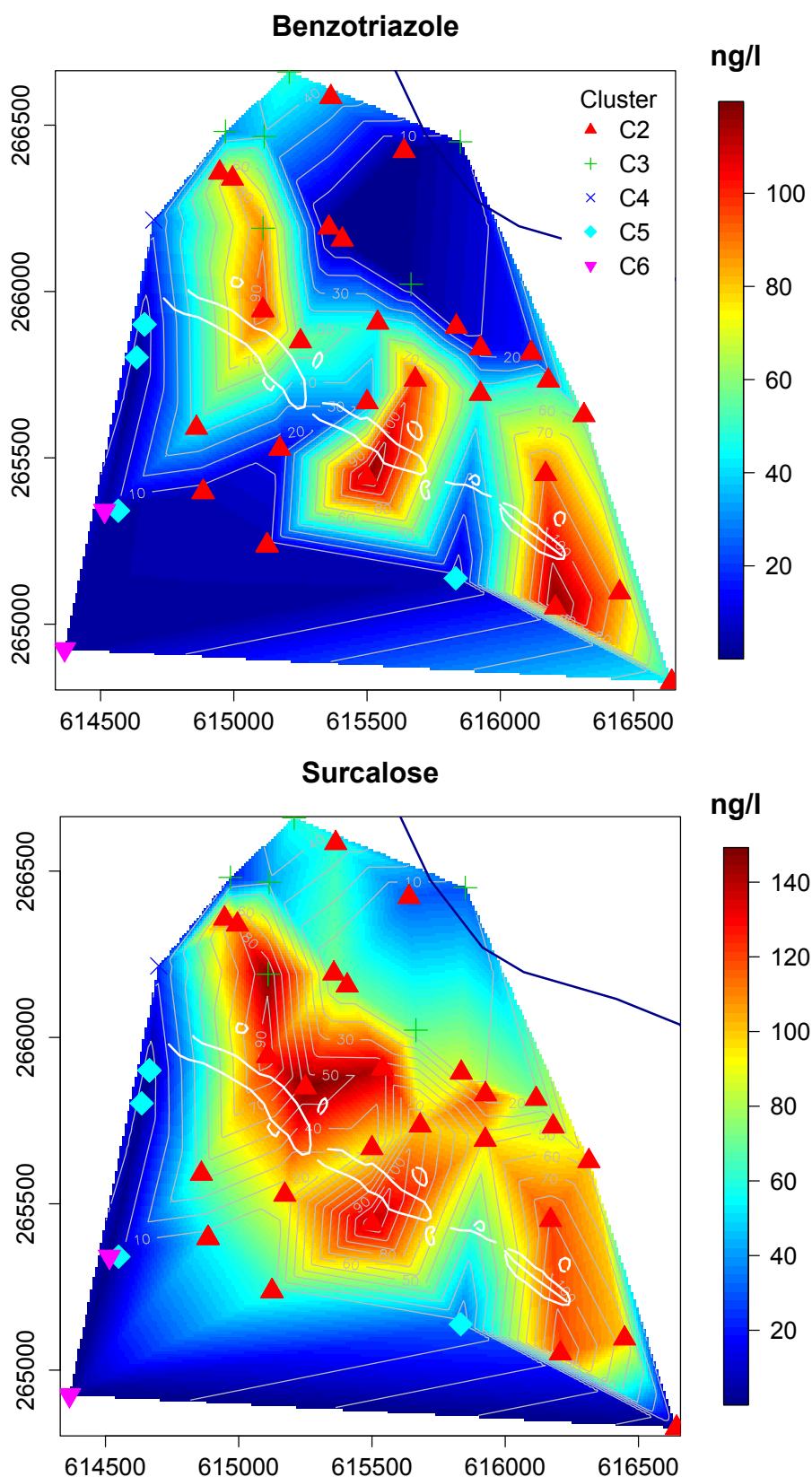


Figure S13: Spatial distribution of benzotriazole (ng/l) and clusters according to the HCA.

Table S1: List of piezometers and wells with coordinates, altitude (masl), relative and absolute depth and reported stratigraphy at the bottom of the well. Na indicates that no information/number are available.

Name	Altitude (masl)	Relativ depth (m)	Absolute depth (m)	Stratigraphy at the bottom of the well	Northing (m)	Easting (m)
21.A.1	269.80	36.90	232.90	Quaternary strata	615266	266137
21.A.10	273.00	41.30	231.70	Quaternary strata	615251	266236
21.A.104	267.25	31.55	235.70	Muschelkalk	616501	265591
21.A.105	275.00	68.30	206.70	Muschelkalk	616448	265095
21.A.11	272.10	39.00	233.10	Quaternary strata	615321	266231
21.A.12	272.08	38.88	233.20	Muschelkalk	615357	266192
21.A.13	273.00	38.51	234.49	Quaternary strata	615407	266156
21.A.14	272.08	38.58	233.50	Muschelkalk	615456	266139
21.A.15	271.90	34.09	237.81	Quaternary strata	615510	266115
21.A.16	272.04	40.94	231.10	Muschelkalk	615551	266088
21.A.17	272.50	41.25	231.25	Quaternary strata	615665	266022
21.A.18	272.81	38.21	234.60	Quaternary strata	615725	266009
21.A.19	272.94	40.19	232.75	Quaternary strata	615752	265951
21.A.20	274.45	40.04	234.41	Quaternary strata	615793	265930
21.A.21	274.20	37.10	237.10	Quaternary strata	615835	265894
21.A.22	273.93	34.21	239.72	Quaternary strata	615880	265860
21.A.23	274.13	35.23	238.90	Jurrasic strat (Opalinuston)	615926	265829
21.A.24	274.83	41.46	233.37	Quaternary strata	616022	265777
21.A.25	273.20	31.80	241.40	Jurrasic strat (Limestone)	616014	265980
21.A.26	274.10	37.70	236.40	Jurrasic strat (Limestone)	616116	265815
21.A.27	274.70	40.45	234.25	Jurrasic strat (Limestone)	616180	265732
21.A.28	274.80	36.30	238.50	Keuper	616226	265673
21.A.29	274.80	37.26	237.54	Muschelkalk	616314	265628
21.A.3	270.79	31.40	239.39	Muschelkalk	614897	266381
21.A.30	271.01	38.80	232.21	Quaternary strata	615363	266069
21.A.31	270.00	34.40	235.60	Quaternary strata	615440	266040
21.A.32	269.53	28.70	240.83	Quaternary strata	615528	265953
21.A.33	272.45	40.21	232.24	Muschelkalk	615110	266190
21.A.34	270.82	45.50	225.32	Quaternary strata	615200	266165
21.A.4	271.35	39.70	231.65	Muschelkalk	614947	266357
21.A.5	270.50	29.20	241.30	Muschelkalk	614995	266339
21.A.6	271.33	31.20	240.13	Dolomitzone	615044	266303
21.A.7	270.00	26.11	243.89	Quaternary strata	615114	266466
21.A.9	272.36	33.20	239.16	Quaternary strata	615201	266285
21.C.16	266.40	25.28	241.12	Sulfate Zone	615639	266422
21.C.18	266.16	38.66	227.50	Sulfate Zone	615364	266584
21.C.206	272.20	29.00	243.20	Muschelkalk	614700	266215
21.C.21	272.90	44.30	228.60	Sulfate Zone	615310	266450
21.C.210	271.69	30.15	241.54	Middle Muschelkalk	615540	265905

21.C.211	270.58	Na	Na	Not available	614636	265802
21.C.213	273.05	17.20	255.85	Jurassic strat (Limestone)	615850	265450
21.C.215	271.83	27.50	244.33	Hauptmuschelkalk	615250	265850
21.C.216	271.78	31.00	240.78	Hauptmuschelkalk	615380	265860
21.C.217	273.50	39.20	234.30	Quaternary strata	615530	266265
21.C.218	272.96	50.00	222.96	Quaternary strata	615905	266035
21.C.219	273.66	20.00	253.66	Muschelkalk	615500	265667
21.C.220	271.36	18.30	253.06	Muschelkalk	614917	266040
21.C.221	273.05	19.20	253.85	Muschelkalk	614890	265833
21.C.222	273.61	19.50	254.11	Muschelkalk	615173	265527
21.C.223	273.28	26.00	247.28	Quaternary strata	615500	265440
21.C.226	275.57	27.60	247.97	Muschelkalk	616590	264935
21.C.227	275.20	27.20	248.00	Hauptmuschelkalk	616523	265206
21.C.228	276.70	28.00	248.70	Quaternary strata	615833	265138
21.C.229	277.80	27.80	250.00	Muschelkalk	616207	265050
21.C.230	274.26	21.10	253.16	Quaternary strata	614798	265416
21.C.231	274.33	21.20	253.13	Muschelkalk	615308	265273
21.C.234	273.70	30.30	243.40	Muschelkalk	615681	265735
21.C.235	274.38	31.50	242.88	Quaternary strata	616170	265451
21.C.237	274.01	21.30	252.71	Muschelkalk	614606	265628
21.C.240	273.35	25.70	247.65	Jurassic strat (Limestone)	614514	266180
21.C.36	262.84	24.30	238.54	Middle Muschelkalk	615208	266660
21.C.43	273.83	32.95	240.88	Jurassic strat (Limestone)	615925	265692
21.C.71	270.02	40.58	229.44	Muschelkalk	614969	266481
21.C.80	273.20	25.70	247.50	Muschelkalk	614860	265590
21.C.81	273.40	23.00	250.40	Muschelkalk	615111	265381
21.J.100.upper	274.81	21.80	253.01	Muschelkalk	614515	265341
21.J.100.middle	274.81	45.20	229.61	Muschelkalk	614515	265341
21.J.100.deep	274.81	76.20	198.61	Middle Muschelkalk	614515	265341
21.J.101.upper	272.90	19.00	253.90	Quaternary strata	614665	265901
21.J.101.middle	272.90	45.20	227.70	Muschelkalk	614665	265901
21.J.101.deep	272.90	76.20	196.70	Muschelkalk	614665	265901
21.J.102.upper	272.40	22.70	249.70	Muschelkalk	615109	265944
21.J.102.middle	272.40	37.00	235.40	Middle Muschelkalk	615109	265944
21.J.102.deep	272.40	47.50	224.90	Sulfate Zone	615109	265944
21.J.103.upper	274.14	20.00	254.14	Muschelkalk	614885	265397
21.J.103.middle	274.14	39.00	235.14	Muschelkalk	614885	265397
21.J.103.deep	274.14	54.00	220.14	Middle Muschelkalk	614885	265397
21.J.104.upper	275.45	27.00	248.45	Muschelkalk	615125	265237
21.J.104.middle	275.45	50.50	224.95	Muschelkalk	615125	265237
21.J.104.deep	275.45	68.00	207.45	Middle Muschelkalk	615125	265237
21.J.89	279.12	70.00	209.12	Keuper	614365	264925
21.J.98.upper	268.80	29.00	239.80	Muschelkalk	616643	264826
21.J.98.middle	268.80	63.50	205.30	Muschelkalk	616643	264826
21.J.98.deep	268.80	80.00	188.80	Middle Muschelkalk	616643	264826

Table S2: List of analysed organic micropollutants from the March sampling campaigns used as indicator substances to indicate the spatial influence of artificial infiltration with surface water for the study area. The descriptive statistics for samples are given in ng/l. Std is the Standard deviation.

Name	CAS-Nr.	Mean	Max	Min	Std
5-Methyl-Benzotriazole	136-85-6	46	140	13	21
Acesulfame	55589-62-3	169	350	48	82
Aliskiren	173334-57-1	25	40	10	11
Amisulpride	71675-85-9	3	4	2	1
Atenolol	29122-68-7	-	-	-	-
Metoprolol acid	56392-14-4	31	51	13	18
Atrazine	1912-24-9	15	32	5	10
Azoxystrobin	131860-33-8	1	1	1	0
Benzotriazole	95-14-7	45	210	0	48
Candesartan	139481-59-7	10	14	3	2
Carbamazepine	298-46-4	12	18	2	4
Carbendazim	10605-21-7	3	7	0	2
Chlortoluron	15545-48-9	1	2	1	0
Clarithromycin	81103-11-9	6	8	3	3
Climbazole	38083-17-9	1	1	1	0
Clothianidin	210880-92-5	-	-	-	-
Coffeine	58-08-2	90	220	28	71
Diclofenac	15307-86-5	24	37	9	14
Diuron	330-54-1	3	11	2	2
Fexofenadine	83799-24-0	-	-	-	-
Fipronil	120068-37-3	-	-	-	-
Hydrochlorothiazid2	58-93-5	10	22	1	6
Ibuprofen	15687-27-1	-	-	-	-
Iopromide	73334-07-3	120	130	110	14

Irbesartan	138402-11-6	6	17	1	6
Isoproturon	34123-59-6	1	2	1	0
Lamotrigine	84057-84-1	15	23	2	4
Mecoprop	93-65-2	-	-	-	-
Metolachlor-ESA	171118-09-5	-	-	-	-
Metoprolol	37350-58-6	8	8	7	1
Oxazepam	604-75-1	4	4	3	1
Sitagliptin	486460-32-6	13	21	4	9
Sucralose	56038-13-2	86	150	18	37
Sulfamethoxazole	723-46-6	16	30	4	6
Terbutylazine	5915-41-3	3	4	2	1
Torasemide	56211-40-6	-	-	-	-
Valsartan	137862-53-4	34	38	30	6
Venlafaxine	93413-69-5	7	14	1	3
Vildagliptin	274901-16-5	-	-	-	-

Table S3: Spatial and temporal standard deviation of major anions and cations for the 85 groundwater sampling locations, where Std is the Standard deviation. In bold red sampling location 21 C.206 is highlighted in red due to a large temporal variation. Furthermore, it identifies Cluster 4, made of only one sample. This cluster differs compared to the other clusters in terms of high concentrations of Na⁺, K⁺ Ca²⁺, Mg²⁺, HCO₃⁻, SO₄²⁻ and Cl. It might be an indication of vertical exchange and upwelling of different waters originating from the salt layer. Rows with NA (Not Available) indicate that a calculation of the standard deviation (Std) was not possible due to only one sample analysed for the considered cat- or anion.

Standard deviation (mg/l)								
-	Na	K	Mg2	Ca2	HCO3	Cl	NO3	SO42
Spatial Std	20.6	0.7	4.9	33.2	89.1	26.8	13.2	32.6
Temporal Std								
<i>Location</i>	Na	K	Mg2	Ca2	HCO3	Cl	NO3	SO42
21.A.1	0.9	0.3	NA	0.4	NA	NA	NA	NA
21.A.10	1.0	0.3	NA	3.3	NA	NA	NA	NA
21.A.104	1.4	0.3	0.7	2.9	10.4	2.8	1.3	NA
21.A.105	10.2	0.4	1.6	3.2	10.3	9.3	2.1	18.2
21.A.11	0.6	0.3	0.1	2.0	2.3	0.8	0.5	NA
21.A.12	0.9	0.2	0.6	4.3	3.6	3.7	1.6	15.2
21.A.13	0.8	0.2	0.4	3.9	3.4	3.3	1.3	14.6

21.A.14	1.0	0.4	NA	0.0	NA	NA	NA	NA
21.A.15	1.0	0.4	NA	0.5	NA	NA	NA	NA
21.A.16	0.7	0.3	0.3	10.2	1.6	3.7	2.3	NA
21.A.17	0.7	0.1	0.4	18.7	3.1	2.6	1.2	1.5
21.A.18	NA	NA	NA	5.6	NA	NA	NA	NA
21.A.19	0.4	0.1	0.0	0.1	NA	3.0	0.9	NA
21.A.20	1.4	0.2	0.6	5.0	4.5	3.4	1.8	NA
21.A.21	1.2	0.2	0.5	2.8	2.8	2.9	1.2	16.9
21.A.22	0.6	0.1	0.2	0.6	1.5	1.2	0.5	NA
21.A.23	0.4	0.2	0.0	2.3	0.5	1.4	0.3	NA
21.A.24	NA	NA	NA	0.8	NA	NA	NA	NA
21.A.25	0.8	0.2	0.7	5.2	8.9	2.2	1.8	NA
21.A.26	0.9	0.1	0.5	3.4	4.2	2.5	1.2	15.1
21.A.27	0.5	0.1	0.1	1.4	2.2	0.0	0.8	NA
21.A.28	0.9	0.1	0.6	4.5	7.3	2.0	1.4	NA
21.A.29	1.0	0.1	0.5	12.2	4.3	2.7	1.2	18.3
21.A.3	2.3	0.3	0.1	9.8	NA	0.7	0.8	NA
21.A.30	0.5	0.0	NA	0.1	NA	NA	NA	NA
21.A.31	1.2	0.3	0.6	3.9	NA	5.3	1.7	NA
21.A.32	2.3	0.3	0.5	8.9	4.2	0.1	1.4	NA
21.A.33	2.4	0.1	0.6	9.0	10.2	4.1	1.5	41.2
21.A.34	0.4	0.1	0.1	3.0	12.5	4.4	1.5	NA
21.A.4	1.4	0.2	0.5	4.4	4.6	3.2	1.2	6.9
21.A.5	0.2	0.2	0.2	9.6	3.3	0.2	0.5	NA
21.A.6	3.6	0.2	0.2	8.7	13.9	3.0	1.4	NA
21.A.7	4.9	0.4	0.5	11.8	11.1	3.6	1.1	13.4
21.A.9	0.8	0.2	0.2	10.8	1.8	4.7	2.0	NA
21.C.16	1.0	0.4	0.6	6.3	6.5	1.2	1.0	31.8
21.C.18	1.7	0.2	1.0	4.8	0.8	1.8	1.9	18.4
21.C.206	80.9	2.1	7.8	77.5	180.5	108.1	1.9	1013.7
21.C.21	11.3	1.3	0.6	6.2	10.8	11.7	0.4	2.7
21.C.210	1.7	0.2	0.7	3.0	3.1	4.4	1.1	2.5
21.C.211	2.2	0.2	1.3	35.9	5.5	17.0	23.4	9.0
21.C.213	0.9	0.3	0.9	3.2	5.6	2.4	0.7	NA
21.C.215	2.1	0.1	0.7	2.8	2.6	4.9	1.2	19.8
21.C.216	1.6	0.2	1.0	7.5	20.1	3.6	1.5	NA
21.C.217	0.4	0.4	0.3	0.5	8.8	1.3	1.9	NA
21.C.218	0.4	0.1	1.4	8.4	8.8	3.6	1.1	NA
21.C.219	2.1	0.2	0.7	5.3	1.4	4.8	1.7	17.4
21.C.220	0.4	0.2	1.0	1.7	3.3	3.0	1.2	NA
21.C.221	1.3	0.2	1.2	7.2	12.5	3.6	1.6	NA
21.C.222	1.3	0.2	0.3	3.1	11.8	3.0	1.1	11.2
21.C.223	2.3	0.2	1.1	7.8	16.7	4.2	1.0	29.0
21.C.226	0.7	0.1	1.2	9.3	4.5	2.3	0.8	NA
21.C.227	1.4	0.1	1.0	3.7	12.9	3.1	1.5	3.4
21.C.228	0.7	0.1	3.1	18.2	27.6	3.4	23.1	21.7
21.C.229	1.9	0.2	0.8	32.8	20.0	3.5	1.7	11.6
21.C.230	0.6	0.1	0.6	4.6	9.0	2.4	1.9	NA
21.C.231	0.6	0.3	1.0	NA	1.3	0.7	0.5	2.1
21.C.234	1.8	0.2	0.9	3.7	18.4	3.5	0.9	27.0
21.C.235	1.0	0.1	1.3	27.3	12.8	3.8	2.2	16.3
21.C.237	3.7	0.6	5.0	27.1	8.4	33.9	22.8	NA
21.C.240	3.4	0.4	2.9	7.7	40.3	26.2	36.8	5.3
21.C.36	3.9	0.6	6.4	2.7	14.2	7.0	8.0	31.6

21.C.43	1.4	0.2	0.9	2.8	13.7	3.2	1.1	2.5
21.C.71	13.6	0.3	0.6	4.4	42.4	15.9	0.3	10.6
21.C.80	0.5	0.1	0.3	2.2	7.1	2.2	0.7	3.2
21.C.81	1.0	0.5	1.5	NA	NA	1.5	0.3	4.0
21.J.100.upper	3.0	0.2	2.8	1.5	7.4	9.2	2.4	22.9
21.J.100.middle	0.1	0.0	0.4	2.3	7.8	0.8	1.5	3.6
21.J.100.deep	2.0	0.2	0.5	0.1	8.7	0.7	0.4	2.6
21.J.101.upper	1.2	0.3	2.1	2.0	16.3	2.0	2.3	26.2
21.J.101.middle	2.9	0.5	1.3	0.9	3.8	3.7	0.3	15.8
21.J.101.deep	1.7	0.2	0.8	1.4	4.0	2.7	1.2	1.5
21.J.102.upper	1.4	0.1	0.4	2.5	4.1	3.7	1.0	14.8
21.J.102.middle	1.9	0.0	0.5	2.7	3.2	3.7	0.9	14.2
21.J.102.deep	1.7	0.1	0.6	3.6	6.0	3.6	1.7	13.3
21.J.103.upper	0.2	0.1	0.3	1.9	0.9	2.0	1.5	7.5
21.J.103.middle	1.1	0.0	1.6	1.0	11.4	1.0	0.6	19.5
21.J.103.deep	1.2	0.1	0.5	5.0	24.7	1.8	0.3	22.9
21.J.104.upper	0.2	0.3	0.7	6.4	24.1	1.8	0.9	31.4
21.J.104.middle	3.0	0.2	0.7	2.2	5.5	4.0	0.3	18.4
21.J.104.deep	1.5	0.1	0.2	0.4	1.3	1.4	0.3	4.4
21.J.89	0.6	0.0	0.7	2.8	6.0	2.5	0.4	15.4
21.J.98.upper	1.1	0.1	0.9	4.6	5.1	3.3	2.2	16.4
21.J.98.middle	0.2	0.1	0.2	1.0	3.5	1.1	0.2	5.1
21.J.98.deep	1.5	0.2	3.4	3.4	13.1	3.3	0.9	34.5

Table S4: Descriptive statistics for the 85 groundwater sampling locations (concentrations in mg/l) where Std is the Standard deviation.

Parameters	Min	Median	Mean	Max	Std	Skeweness
Na ⁺	3.3	8.7	12.3	105.2	13.18	5.1
K ⁺	0.6	1.7	1.8	4.5	0.58	2.7
Mg ²⁺	5.0	8.7	10.4	33.6	4.74	2.9
Ca ²⁺	26.5	62.4	75.0	165.9	29.18	1.7
HCO ₃ ⁻	169.7	191.1	227.8	502.3	80.85	2.0
Cl ⁻	5.0	13.6	18.7	152.2	18.69	4.9
NO ₃ ⁻	0.8	7.9	11.2	71.1	10.61	3.5
SO ₄ ²⁻	3.1	28.3	39.4	180.9	28.26	2.9
Li ⁻	0.0022	0.0031	0.0075	0.1636	0.02	7.5
Sr ²⁺	0.1320	0.3618	0.3679	1.0557	0.13	2.6
As ³⁺	0.0002	0.0008	0.0008	0.0037	0.00	2.6
U ⁶⁺	0.0001	0.2942	0.3407	0.9210	0.30	0.4

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