Supplement of Hydrol. Earth Syst. Sci., 22, 4401–4424, 2018
https://doi.org/10.5194/hess-22-4401-2018-supplement

Hydrology and Earth System Sciences
Open Access
EGU

Supplement of

Detecting dominant changes in irregularly sampled multivariate water quality data sets

Christian Lehr et al.

Correspondence to: Christian Lehr (lehr@zalf.de)

Table S1. Stream water sampling sites. The abbreviation in the ID refers to the corresponding catchment. N: number of samples.

ID	N	Easting	Northing	Catchment
D_112	126	3426969	5916330	Dauergraben
U_128	114	3423416	5907370	Ucker
St_133	124	3420262	5891835	Stierngraben
S_118	118	3421173	5907839	Strom
S_120	1	3418025	5906225	Strom
S_121	23	3416348	5905013	Strom
S_122	1	3412048	5903419	Strom
Q_93	126	3422251	5908887	Quillow
Q_95	125	3420582	5910416	Quillow
Q_96	11	3420084	5913122	Quillow
Q_97	126	3419850	5913404	Quillow
Q_98	127	3417941	5913091	Quillow
Q_100	110	3412572	5912708	Quillow
Q_104	71	3409712	5912268	Quillow
Q_106	12	3406372	5912814	Quillow
Q_102	11	3410569	5911755	Quillow
Q_103	8	3408376	5910401	Quillow
P_107	78	3410047	5912392	Peege
P_108	61	3408727	5914397	Peege
P_109	8	3410232	5916180	Peege
P_110	51	3410858	5917416	Peege

Table S2. Sampling sites for groundwater quality and groundwater level. The abbreviation in the ID refers to the corresponding catchment. The subscripts Gs = shallow groundwater and Gd = deep groundwater give additional information on the respective groundwater layer. All groundwater wells are inside the Quillow catchment. N: number of samples.

ID	N	Easting	Northing	Depth of screen m (a.s.l)	Depth of screen m below ground
Gd_205	2	3416412	5911941	40.55 - 38.55	15 - 17
Gd_204	25	3412546	5912702	49 - 47	16 - 18
Gs_200	6	3410020	5912439	74.10 - 73.10	4.0 - 5.0
Gs_199	18	3409934	5912302	72.20 - 71.20	3.0 - 4.0
Gd_198	28	3409934	5912302	51.27 - 53.27	22 - 24
Gs_202	11	3409863	5912702	74.14 - 73.14	4.0 - 5.0
Gd_201	25	3409863	5912702	65.79 - 63.79	12.5 - 14.5
Gd_203	25	3409764	5912942	63.46 - 61.46	16 - 18

Table S3. Measurement details of the analysed variables. Before the data analysis NH_4^+ was calculated from NH_4-N, PO_4^{3-} from o-PO_4-P, and the concentration of HCO_3^- was converted from mmol L^{-1} to mg L^{-1}.

Abbreviation	Parameter	Unit	Measuring accuracy; detection limit	missing values in %	n samples < detection limit in %
Stream water and groundwater					
pH	pH value		0.01	0	0
Eh	Redox potential	mV	1	0.57	0
EC	Electric conductivity	µS cm^{-1}	1	0	0
Temp	Water temperature	°C	0.1	0	0
O_2	Oxygen	mg L^{-1}	0.1	1.91	0.25
NH_4-N	Ammonium nitrogen	mg L^{-1}	0.01	0.57	0.76
o-PO_4-P	Phosphorus of orthophosphate	mg L^{-1}	0.01	0	37.53
DOC	Dissolved organic carbon	mg L^{-1}	0.05	3.44	0
Anions					
Cl^-	Chloride	mg L^{-1}	0.03	0	0
NO_2^-	Nitrite	mg L^{-1}	0.03	2.54	65.52
NO_3^-	Nitrate	mg L^{-1}	0.03	0.38	2.93
SO_4^{2-}	Sulfate	mg L^{-1}	0.02	1.34	0
Cations					
Na^+	Sodium	mg L^{-1}	0.01	0	0
K^+	Potassium	mg L^{-1}	0.02	0	0
Mg^{2+}	Magnesium	mg L^{-1}	0.02	0	0
Ca^{2+}	Calcium	mg L^{-1}	0.03	0	0
Only groundwater					
Fe^{2+}	Iron(II)	mg L^{-1}	0.03	0	8.57
HCO_3^-	Hydrogen carbonate	mmol L^{-1}	0.01	6.43	0

Table S4. Site-specific cumulated R^2 of the reproduction of the interpoint distances of the data in the projection by the first four components of Isomap at sites with n > 15. Labels: P, Peege; Q, Quillow; S, Strom; St, Stierngraben; U, Ucker; D, Dauergraben; Gs, shallow groundwater; Gd, deep groundwater.

ID	Gd_203	Gd_201	Gd_198	Gd_204	Gs_199	P_110	P_108	P_107	Q_104	Q_100
N	25	25	28	25	18	51	61	78	71	110
Cp. 1	0.1	0.62	0.01	0.15	0.01	0.25	0.36	0.11	0.21	0.27
Cp. 2	0.33	0.69	0.25	0.33	0.08	0.38	0.46	0.27	0.33	0.61
Cp. 3	0.49	0.79	0.6	0.5	0.2	0.45	0.56	0.53	0.41	0.64
Cp. 4	0.5	0.8	0.74	0.55	0.29	0.59	0.97	0.65	0.74	0.8

ID	Q_98	Q_97	Q_95	Q_93	S_121	S_118	St_133	U_128	D_112
N	127	126	125	126	23	118	124	114	126
Cp. 1	0.33	0.36	0.2	0.11	0.35	0.15	0.3	0.11	0.54
Cp. 2	0.43	0.46	0.31	0.24	0.43	0.25	0.45	0.27	0.64
Cp. 3	0.59	0.58	0.35	0.3	0.68	0.39	0.59	0.4	0.73
Cp. 4	0.72	0.66	0.67	0.72	0.66	0.7	0.67	0.52	0.83

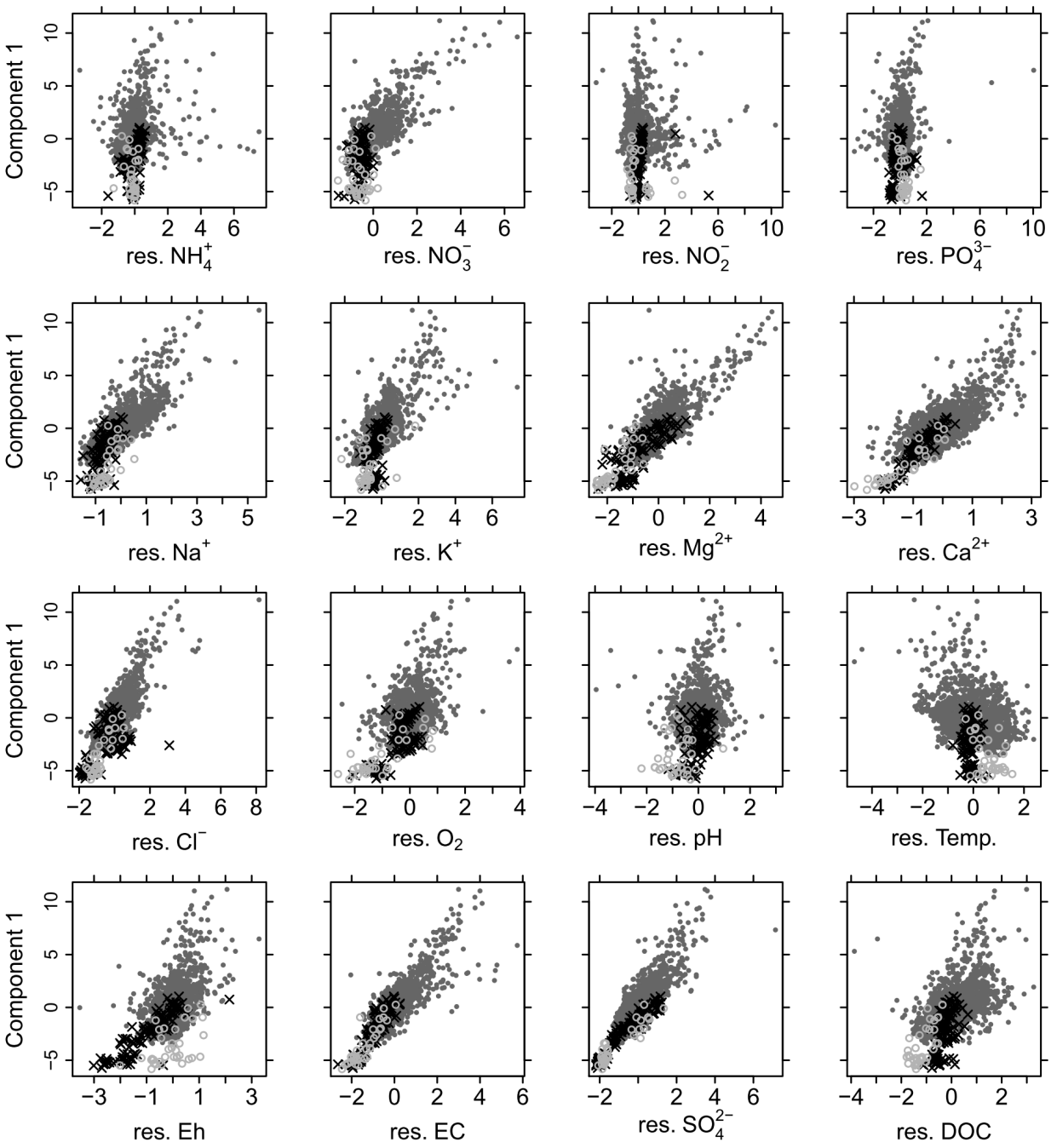

Figure S1. Residuals of the multiple linear regression of selected single variables and component 2-4 versus scores of component 1. Grey filled dots: stream water. Light grey open circles: shallow groundwater. Black x-mark: deep groundwater.

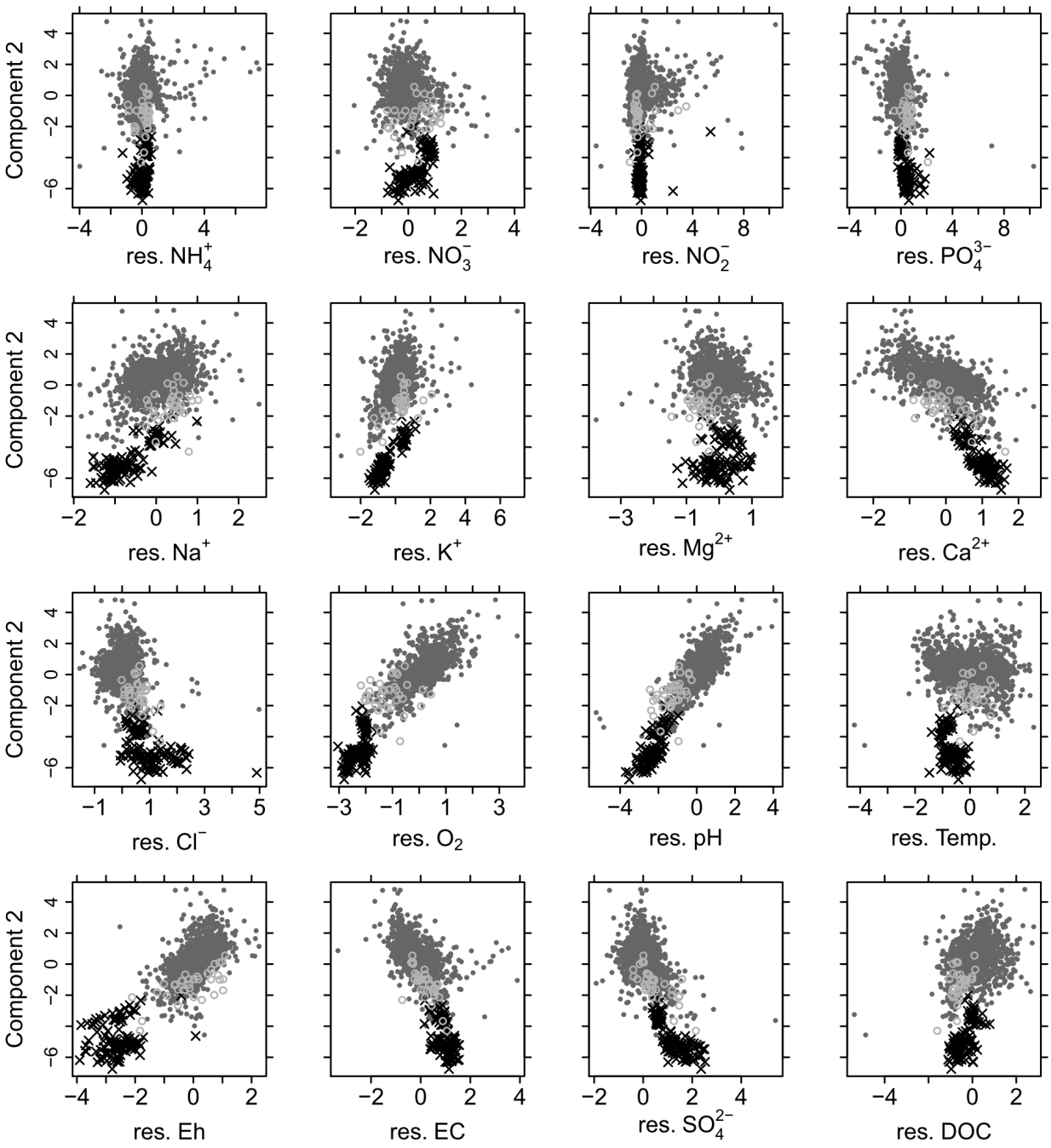

Figure S2. Residuals of the multiple linear regression of selected variables on component 1, 3 and 4 versus scores of component 2. Grey filled dots: stream water. Light grey open circles: shallow groundwater. Black x-mark: deep groundwater.

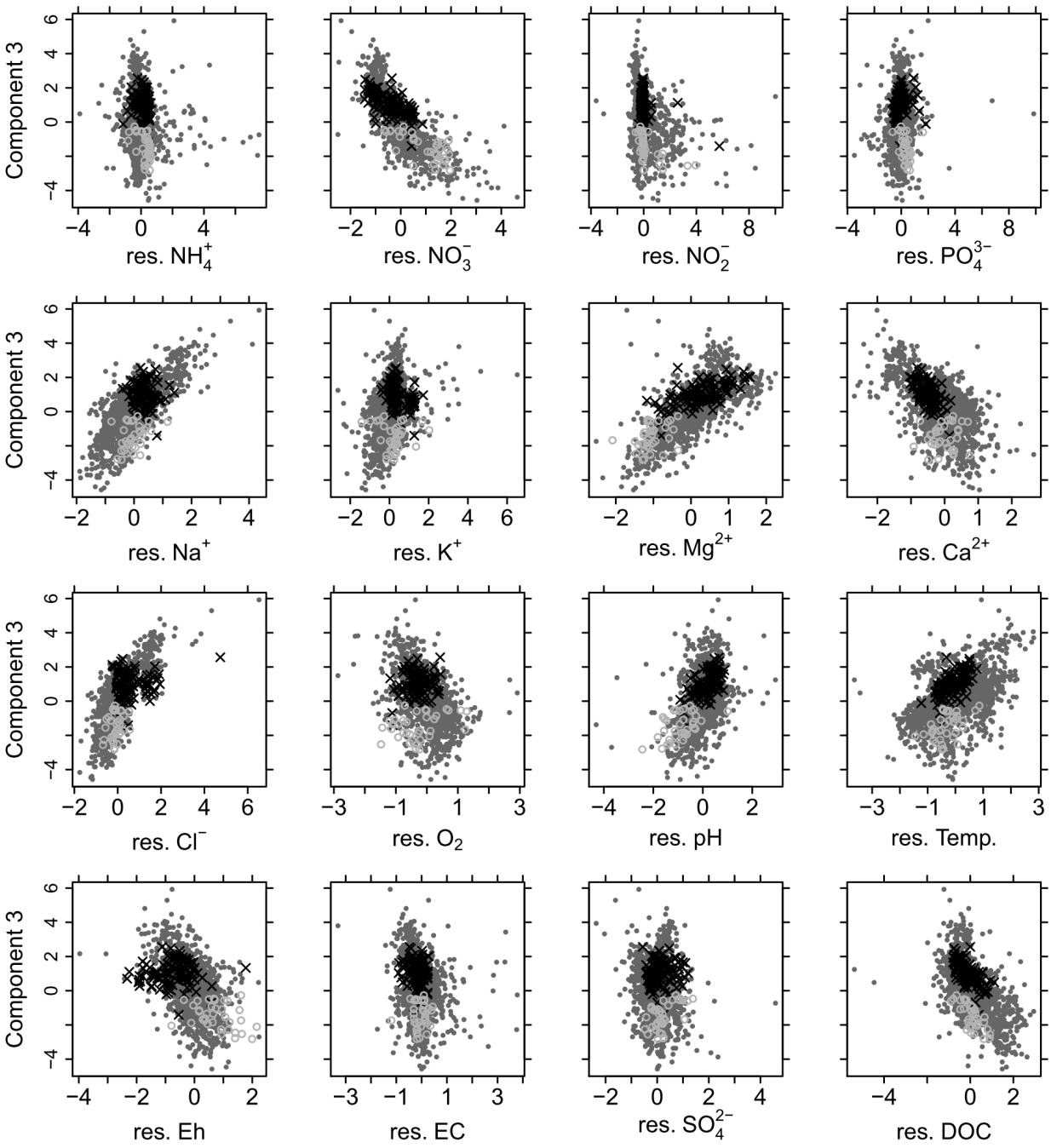

Figure S3. Selection of residuals of the multiple linear regression of single variables and component 1, 2 and 4 versus scores of component 3. Grey filled dots: stream water. Light grey open circles: shallow groundwater. Black x-mark: deep groundwater.

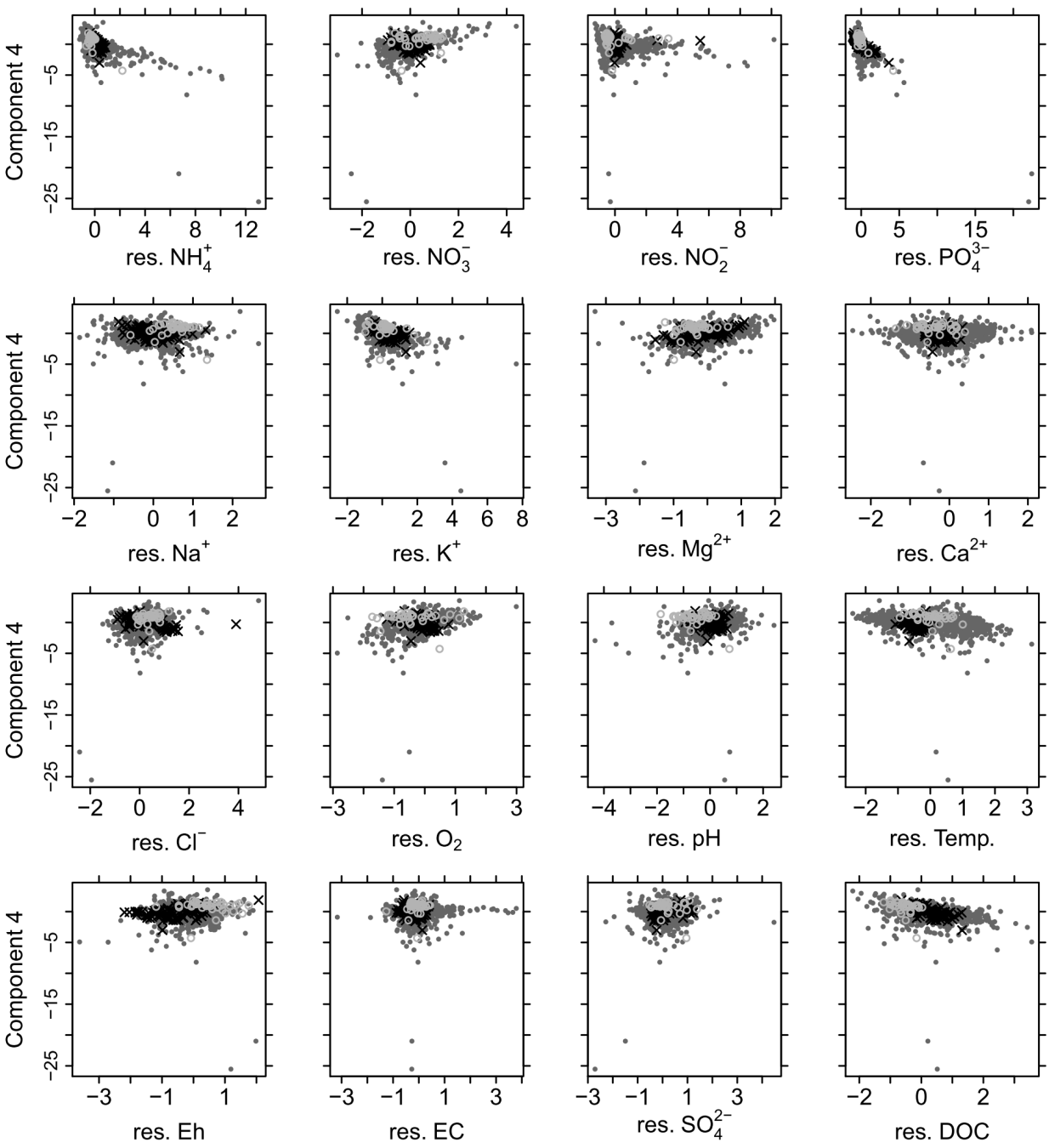

Figure S4. Selection of residuals of the multiple linear regression of single variables and component 1-3 versus scores of component 4. Grey filled dots: stream water. Light grey open circles: shallow groundwater. Black x-mark: deep groundwater.