Supplementary Materials of A Novel Method for Determination of the Natural Toxin Ptaquiloside in Ground and Drinking Water

Water chemistry data for raw groundwater and treated water from study site Vigersted

Table S1. Water chemistry data for raw groundwater and treated water (Vigersted) sampled in January 2019. Source: HOFOR (Denmark).

Parameter	Vigersted (raw water)	Vigersted (treated water)	Unit
Total alkalinity	6.5	6.0	mmol L^{-1}
Hardness (total)	19.3	20.2	° dH
Sodium	60	66	mg L^{-1}
Magnesium	17	21	mg L^{-1}
Calcium	110	110	mg L^{-1}
Manganese	0.073	0.001	mg L^{-1}
Iron	1.7	0.01	mg L^{-1}
Zinc	1.1	0.59	µg L^{-1}
Chromium	0.056	0.010	µg L^{-1}
Cadmium	0.0030	0.0072	µg L^{-1}
Nickel	0.52	0.030	µg L^{-1}
Cobalt	0.030	0.017	µg L^{-1}
Arsenic	0.13	0.14	µg L^{-1}
Potassium	5.8	5.4	mg L^{-1}
Oxygen	0.04	10.7	mg L^{-1}
Selenium	0.050	0.10	µg L^{-1}
Phosphorus (total)	0.036	0.003	mg L^{-1}
Chloride	94	110	mg L^{-1}
Carbonate	2	2	mg L^{-1}
Bicarbonate	400	370	mg L^{-1}
Hydrogen sulfide	0.02	0.02	mg L^{-1}
Sulphate	52	60	mg L^{-1}
Methane at 10 ° C	0.045	0.010	mg L^{-1}
Ammonia + ammonium	0.85	0.004	mg L^{-1}
Nitrate	0.10	1.5	mg L^{-1}
Nitrite	0.0010	0.0020	mg L^{-1}
NVOC (non-volatile organic carbon)	3.2	2.6	mg L^{-1}

Map of the study site (Vigersted) and Humleore forest

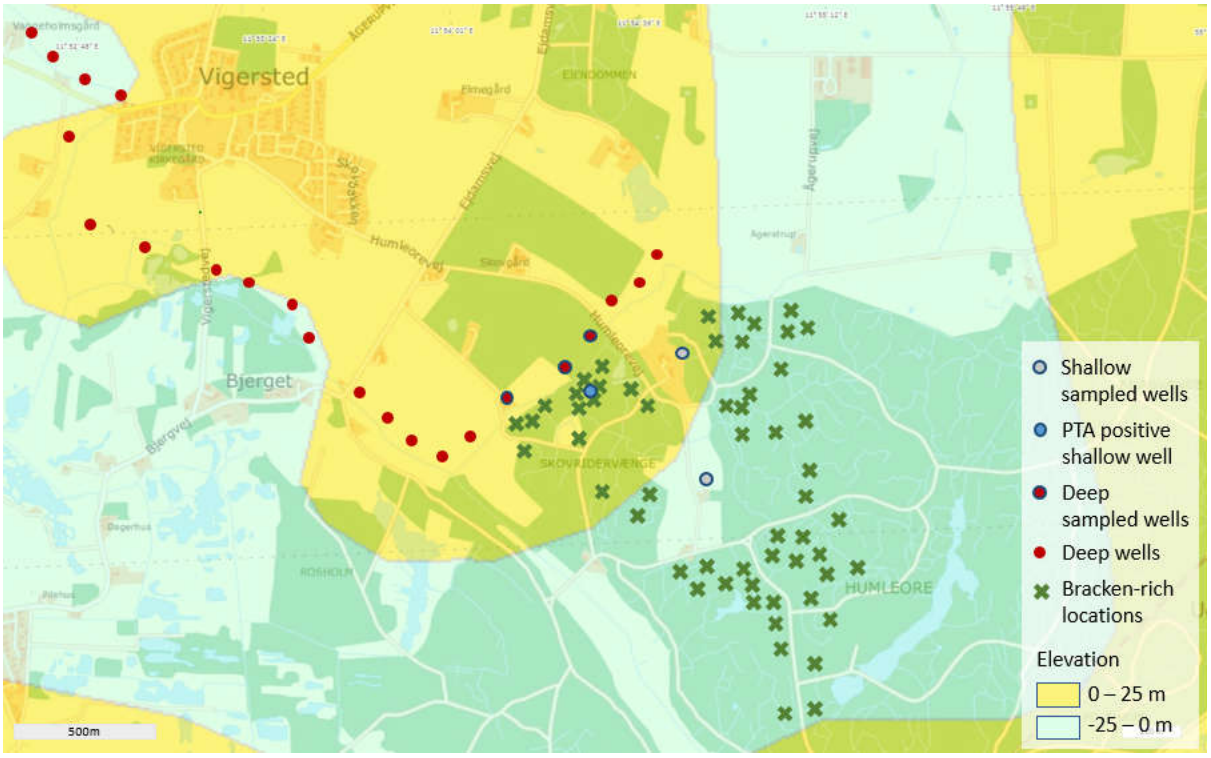

Figure S1. Vigersted water wells field site, water wells included in the monitoring and bracken-rich area in Humleore forest. Source: GEUS database, Denmark [47].

Development of the PTA preservation method by applying Plackett-Burman experimental design

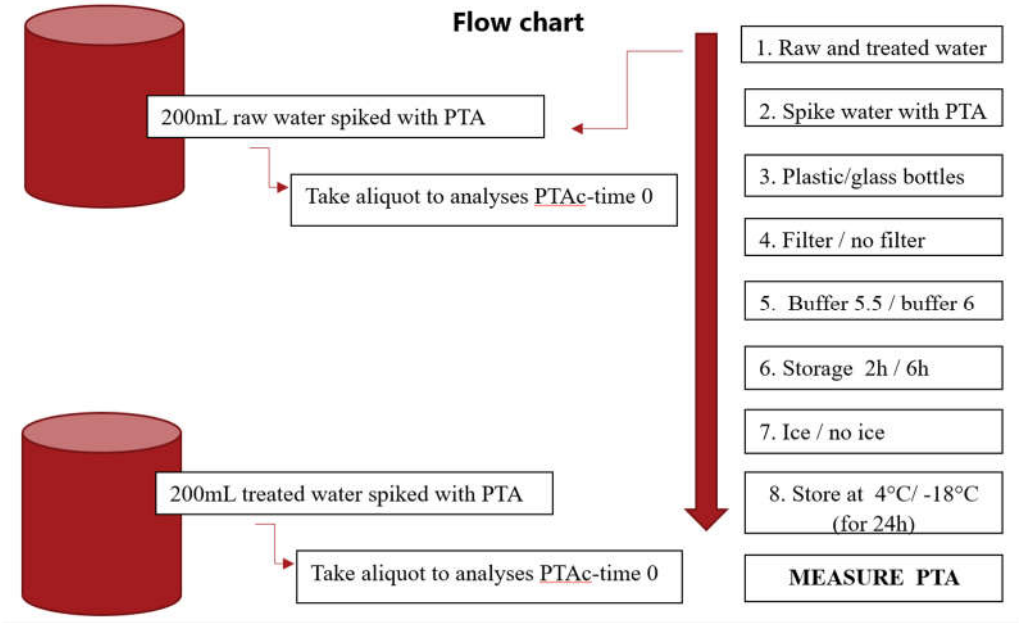

Figure S2. Flow chart for developing the preservation method of PTA in groundwater samples.

Validation of the analytical method (LC-MS) - Linearity of calibration curves over investigated concentration ranges

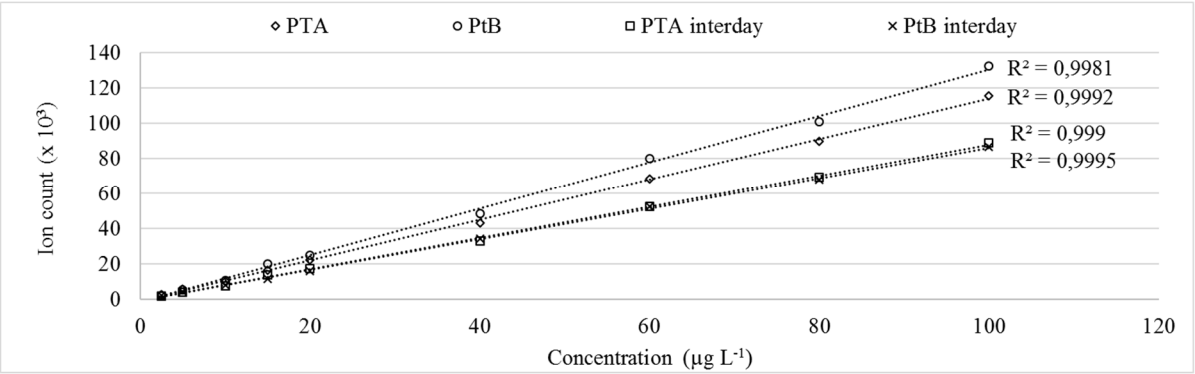

Figure S3. Calibration curves of the standard solutions of analytes.

Calibration curves in Figure S3 are produced for validation of LC-MS method described in Rai et al. [43]. Each calibration curve was made from 10 data points. Intraday measurements of both PTA and PtB were taken.