

# Does the Natural Carcinogen Ptaquiloside Degrade Readily in Groundwater?

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## Research

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## Abstract

Background: Ptaquiloside (PTA) is a natural carcinogen found in bracken ferns. PTA is released from the plants via soil to surface and groundwaters from where humans can be exposed via drinking water. Primary degradation of PTA is due to hydrolysis with formation of pterosin B (PTB). Temperature and pH determine the rate of hydrolysis under pure experimental conditions. To assess the applicability of the experimental model to natural groundwaters, PTA degradation kinetics were examined in a range of natural groundwaters at environmentally relevant conditions.

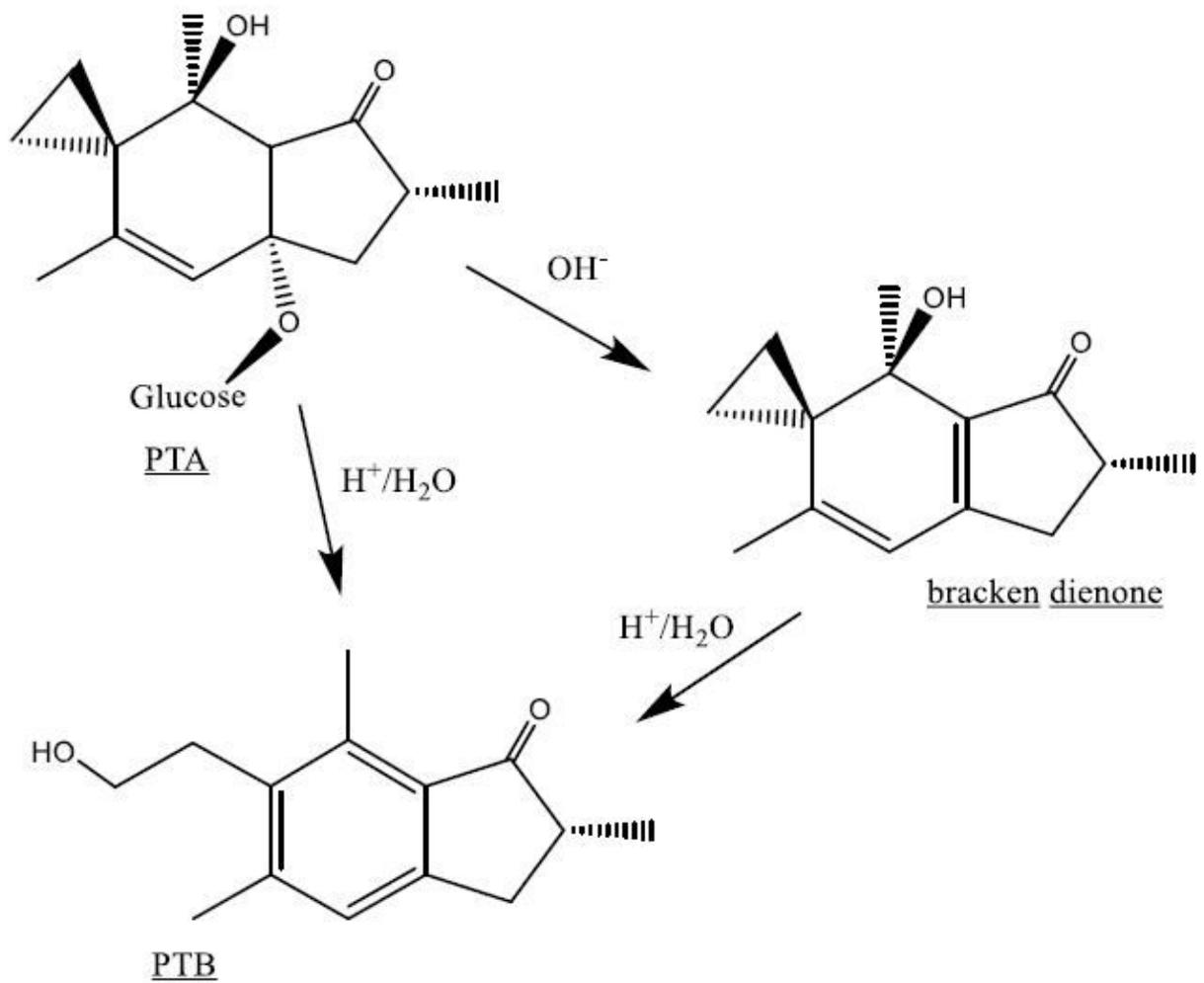
Results: PTA was quantified by UPLC-MS/MS. Over an 80-day study period, PTA half-lives ranged from 6.5 to 47 days (natural pH; 8.0oC). The fastest degradation was observed for the most alkaline groundwaters with pH of around 8. Rates of degradation was well predicted using an existing rate equation for hydrolysis. However, deviations from this model were found, especially at the extremes of the examined pH-range (4.7-8.2). The rate of conversion of PTA to PTB was close to unity around neutral pH. However, at slightly acidic conditions, formation of PTB could only count for 9% of the degraded PTA, indicating formation of other products.

Conclusions: Degradation of PTA in groundwater is determined by pH and temperature, and PTA can prevail for months under slightly acid to neutral pH conditions. The existing laboratory-based model for PTA hydrolysis is generally applicable for groundwaters but needs further validation at high and low pH.

## Full Text

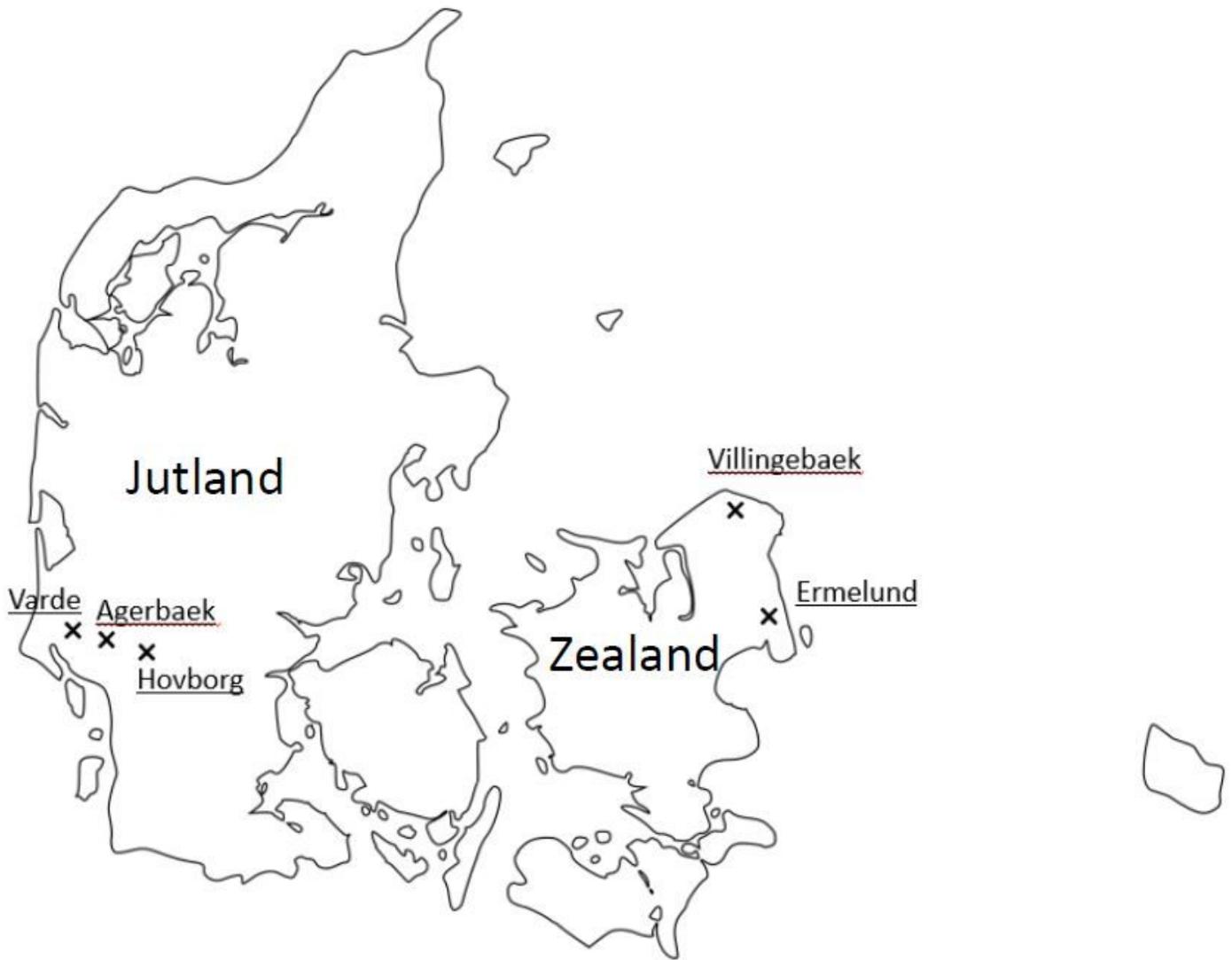
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## Figures



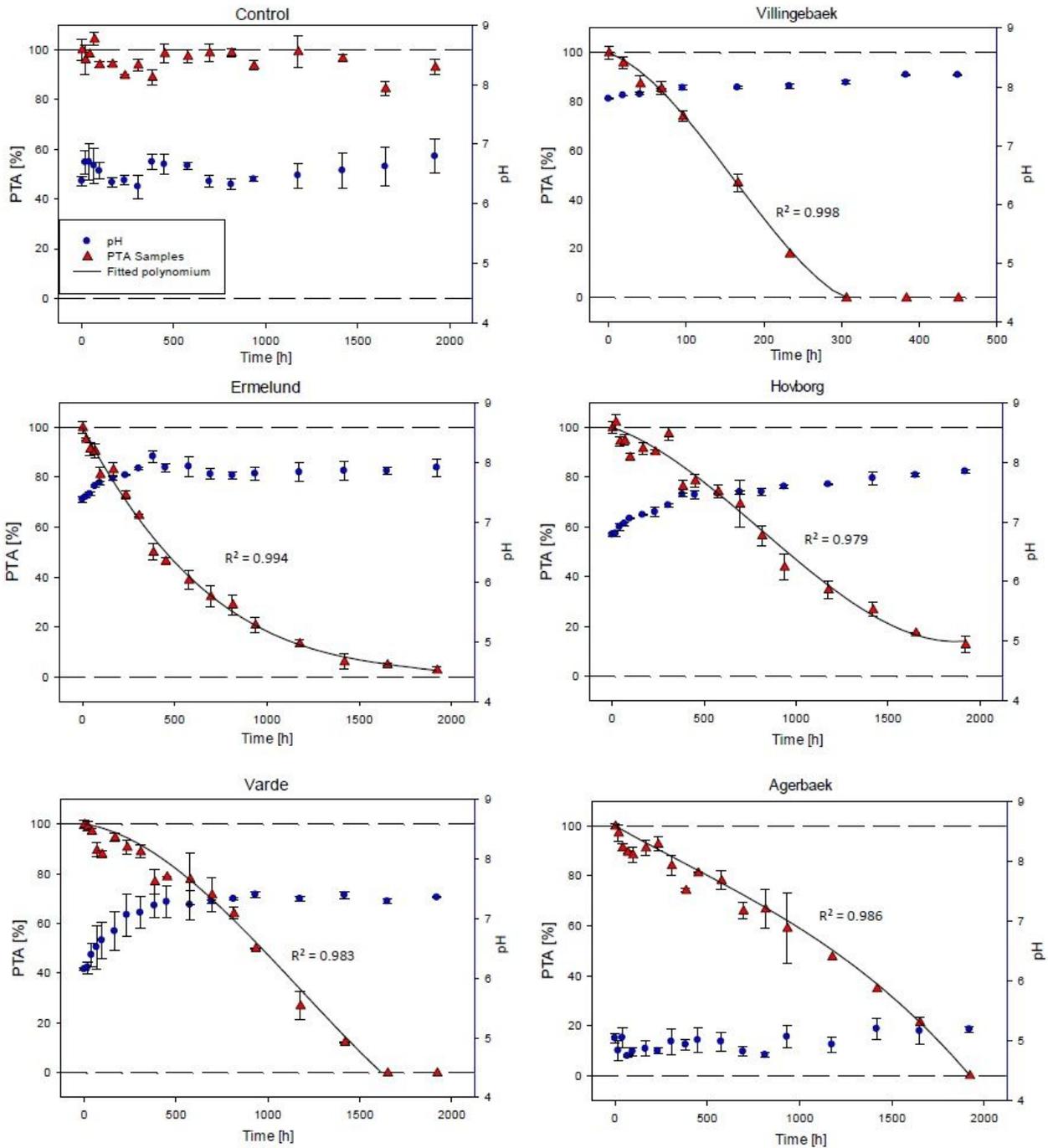
**Figure 1**

Hydrolysis of ptaquiloside (PTA) and formation of the main metabolites pterosin B (PTB) and the bracken dienone under alkaline and/or acidic conditions. Other metabolites and reaction intermediates may form depending on reaction conditions. Adapted from [1].



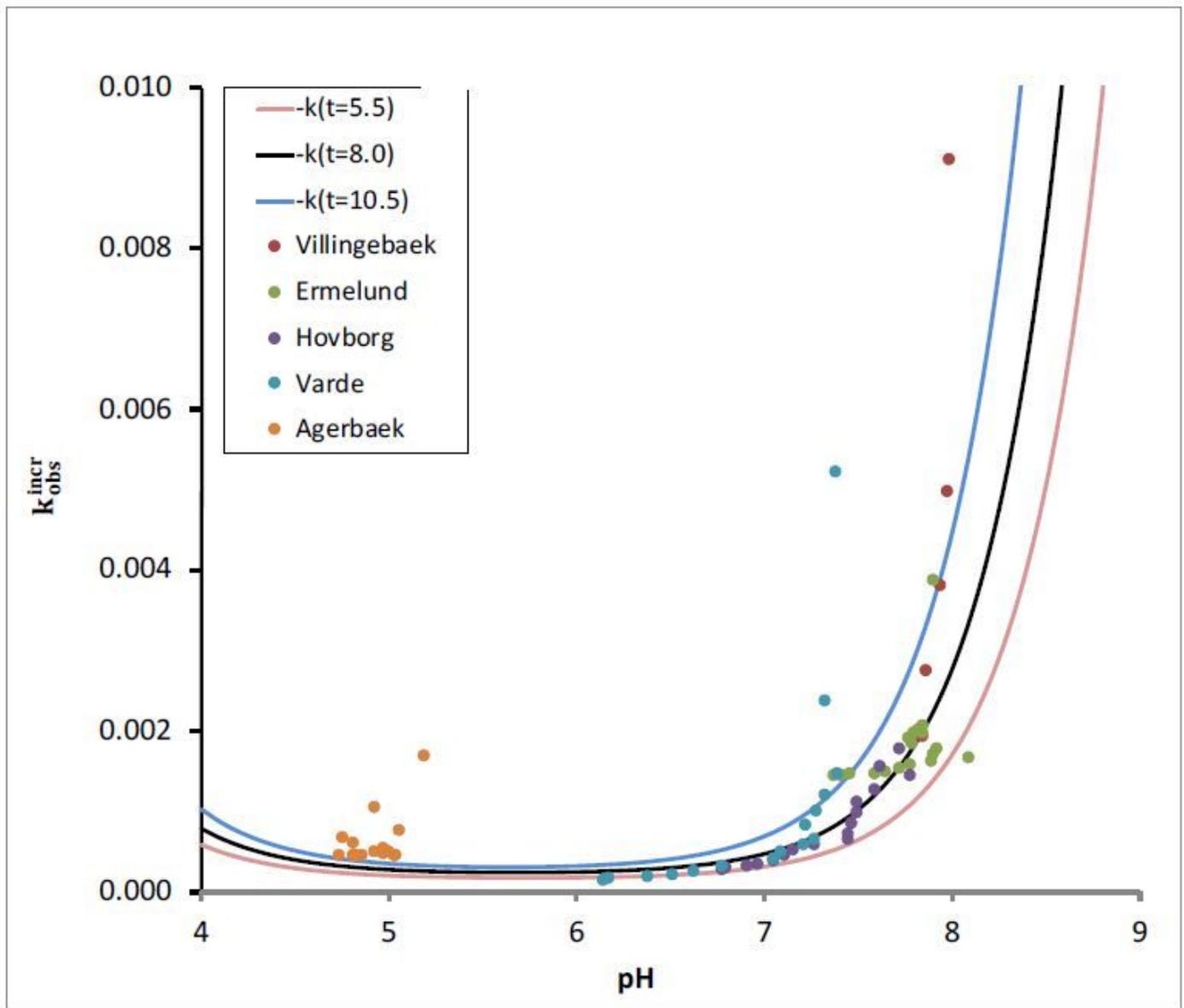
**Figure 2**

Map of Denmark with the five groundwater sampling locations (water plants).



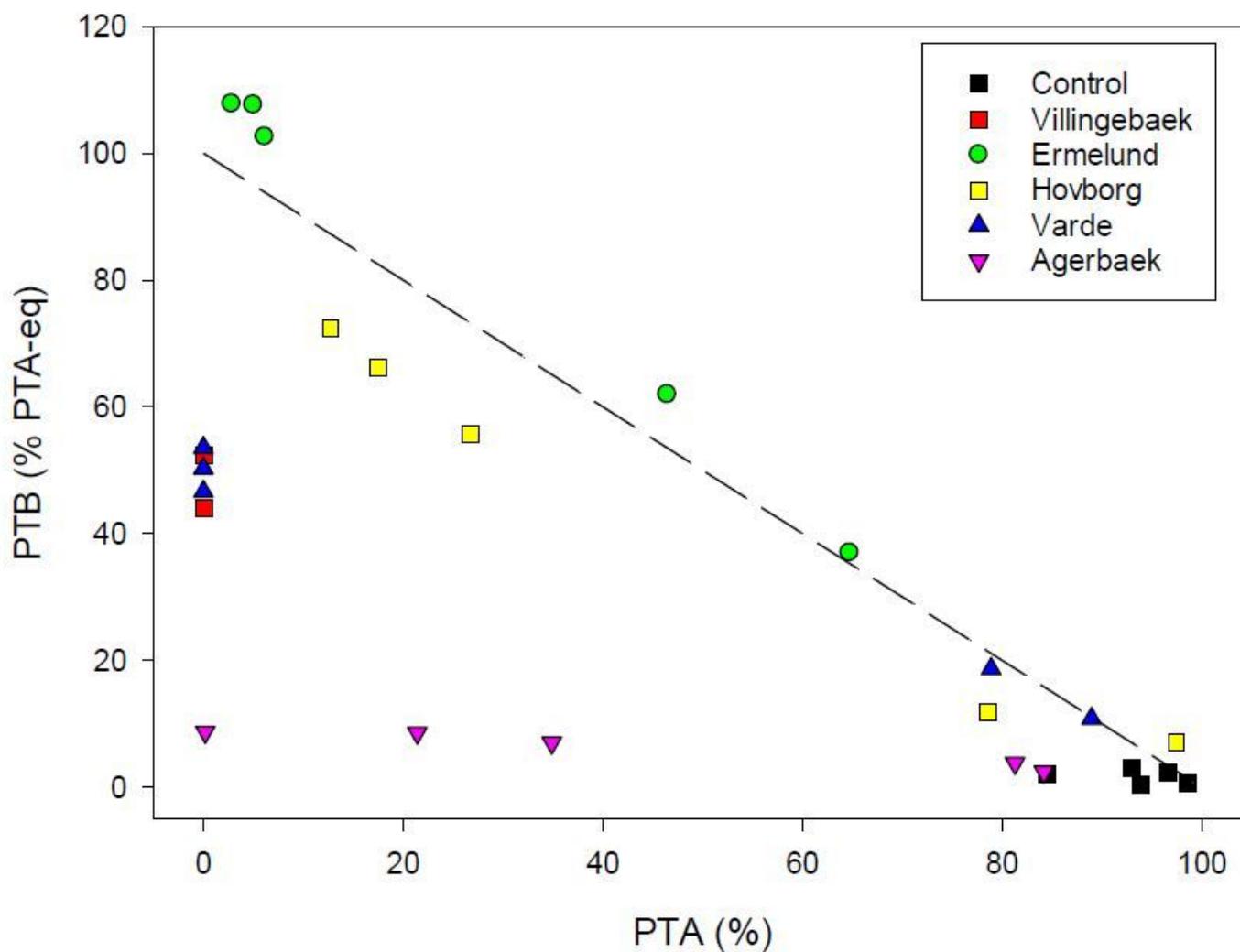
**Figure 3**

Relative PTA concentration versus time in PTA-groundwater hydrolysis experiments (red triangles) and the corresponding fits with a 3rd degree polynomial (Eq. 2; goodness of fit  $R^2$ ), except from Control where no significant degradation took place. Development in pH (blue). Note the short time scale for Villingebaek (fast disappearance of PTA). Error bars show the standard deviation ( $n=3$ ).



**Figure 4**

Observed degradation constant ( $k_{obs}^{incr}$ ) versus pH in groundwaters. Filled circles represent measured data. Curves show predicted degradation rates from Ayala-Luis et al. [17] at temperatures 5.5, 8.0 and 10.5 °C corresponding to experimental conditions. Measurements above the line indicate faster degradation rates than expected and below the line indicate slower degradation rates than expected.



**Figure 5**

PTB vs. PTA detected in samples at different time points in the degradation experiment relative to the concentration at start for each of the waters. The solid line marks a 1:1 conversion from PTA to PTB. Relative standard deviation (quality control standards) was < 7 %.

## Supplementary Files

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- [Supplementarymaterial6.pdf](#)