Are PMOCs less toxic?

Linking physicochemical compound properties with measured toxicity

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Background

Persistent and mobile organic chemicals (PMOCs) are gaining attention as a potential threat to the quality of water resources.[1] Due to their high persistence and mobility they evade water treatment processes and persist and accumulate in water cycles, leading to human- and environmental exposures to PMOCs.[2] But, does their high mobility make them inherently less toxic than their hydrophobic counterparts?

Aim

To gain insight into the toxicity and toxic mechanisms relating to the physico-chemical properties that determine chemical persistence and mobility in water

Methods

1. **Physicochemical database** for 3360 water-relevant chemicals matched with their activity in 534 ToxCast assays
2. **Random forest analysis** to identify chemical properties that correlate with effects
3. **Regression analyses** to quantify the strength and direction of relationships

Results & Discussion

- Random forest showed that polarity (K_{OW} & K_{OC}) is inversely related to effect concentrations (Fig. 1)
- Only weak negative relations were observed using linear regressions (Fig. 2)
- Some toxic mechanisms are more defined by mobility than others, providing insight for (prospective) risk assessment

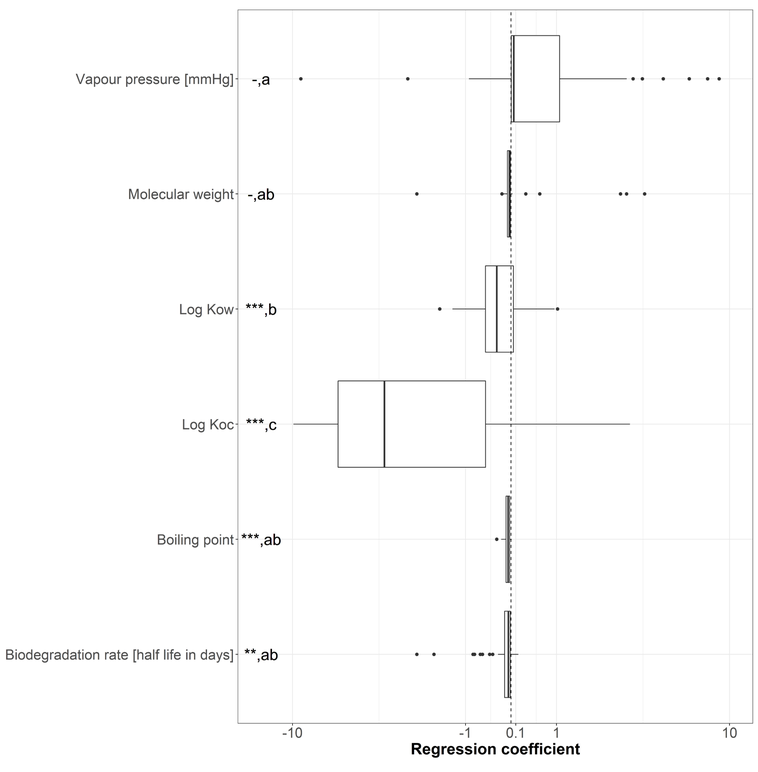
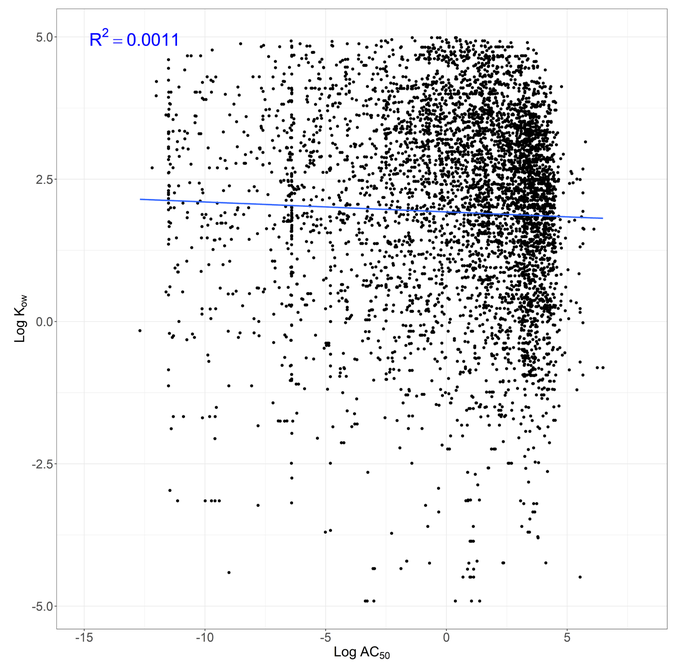
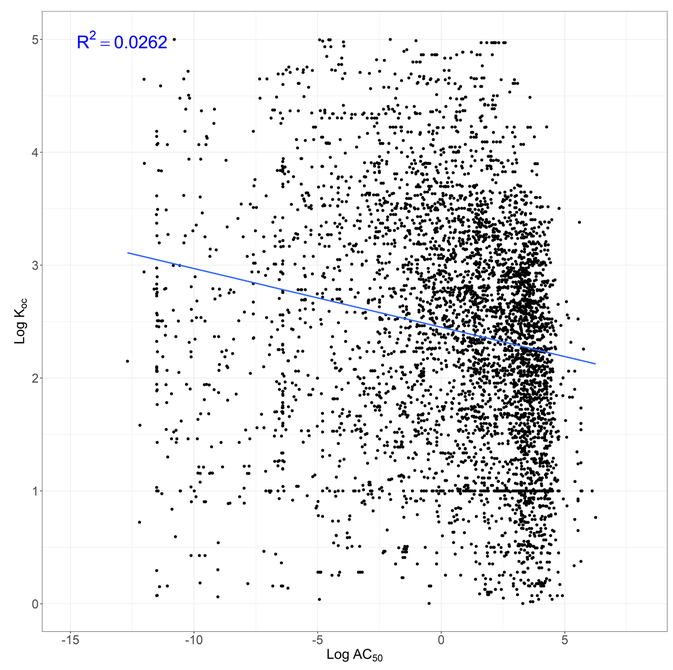


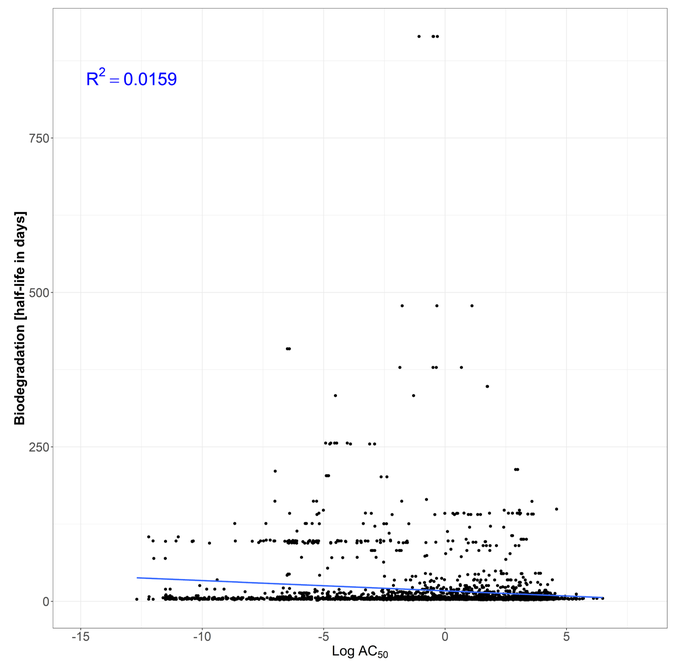
Figure 1 Regression coefficients from a random forest analysis of 113 toxicity tests for the toxicity of water-relevant chemicals with physicochemical properties related to their mobility in water. ***; $\mu \neq 0$, $p < 0.001$, **; $\mu \neq 0$, $p < 0.01$, *; $\mu \neq 0$, $p < 0.05$, -; $\mu = 0$, $p > 0.05$. Letters indicate significantly similar regression coefficient distributions.



Octanol-water partition coefficient (K_{OW})



Organic carbon-water partition coefficient (K_{OC})



Biodegradation

Figure 2 Linear regression analyses for effect concentrations (AC_{50}) of water-relevant chemicals with their octanol-water (K_{OW}) and organic carbon-water (K_{OC}) partition coefficients, and their biodegradation rates.

Conclusions

PMOCs appear to be inherently less toxic, but their diversity and pervasiveness in water cycles warrant further investigations into their threat to water quality

References
1. Hale et al. 2022, Environ. Sci. Eur. 34 (1), 1-24
2. Reemtsma et al. 2016, Environ. Sci. Technol. 50, 19, 10308-10315