Hydrolysis and biotransformation-derived persistent and mobile organic contaminants potentially impacting raw and drinking waters

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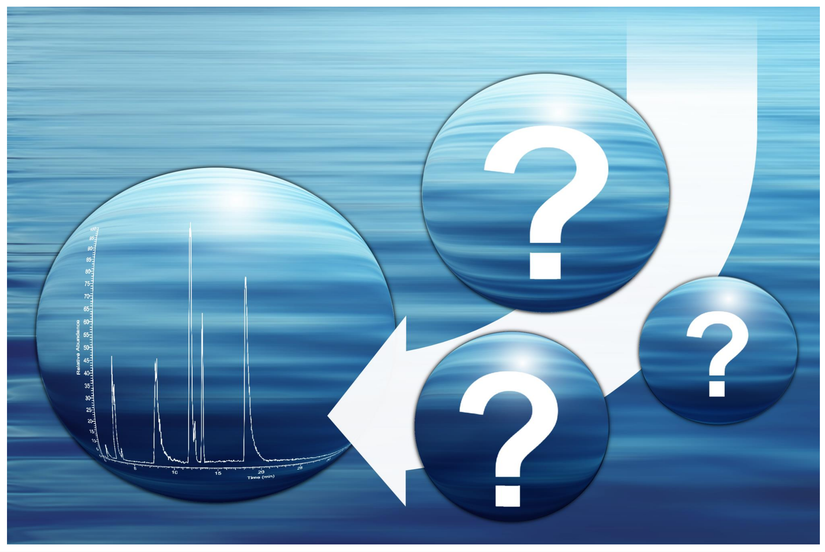
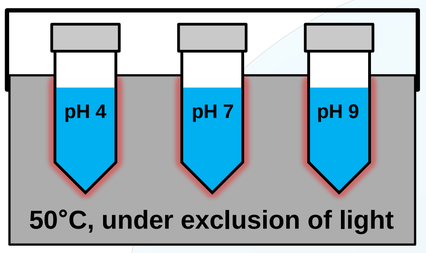
Introduction

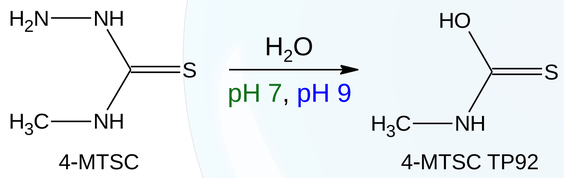
Persistent and mobile organic contaminates (PMOC) are able to penetrate natural and artificial barriers, spread along the water cycle, and potentially even **reach drinking water**. Many PMOC are assumed to be **highly polar** and thus outside the well investigated polarity range in environmental chemistry[1]. As a consequence a large fraction of PMOC may still be unknown.

Recent non-target[2] and suspect screenings[3] for very polar substances led to the discovery of several novel water contaminants. To further extent our knowledge of potentially drinking water relevant PMOC in preparation of an extended monitoring campaign, we studied the transformation of **predicted PMOC precursors** with a high chance of emission into the environment and included the transformation products (TPs) in a previously developed UHPLC-HILIC-sMRM method.

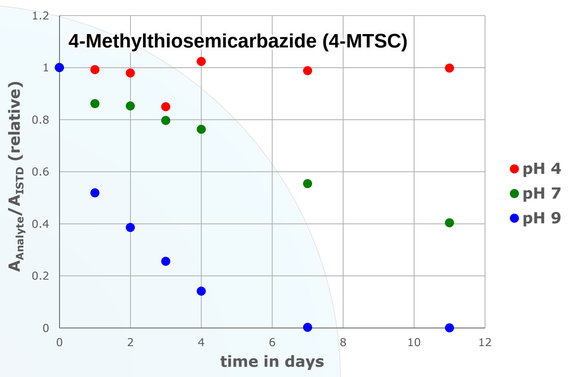
Which chemicals may contaminate our drinking water?

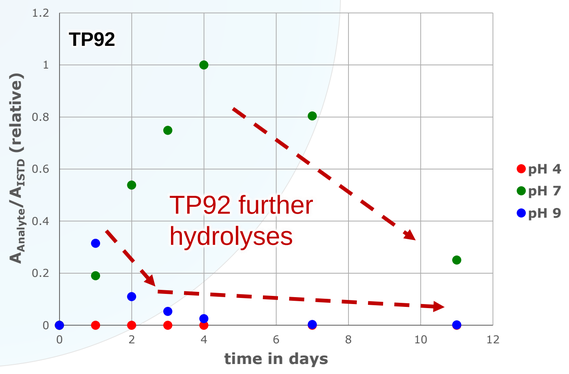




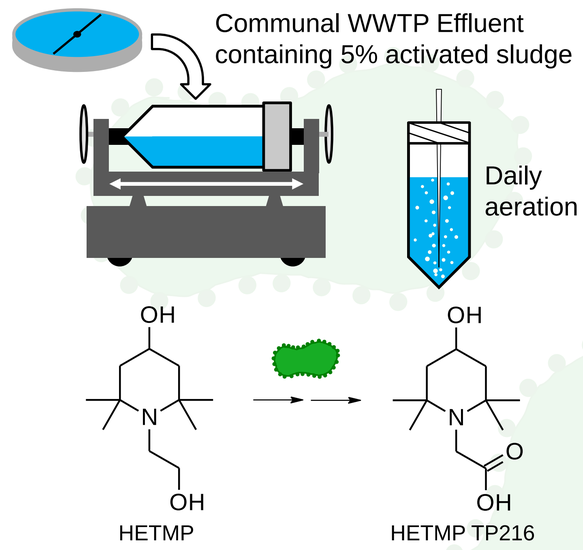


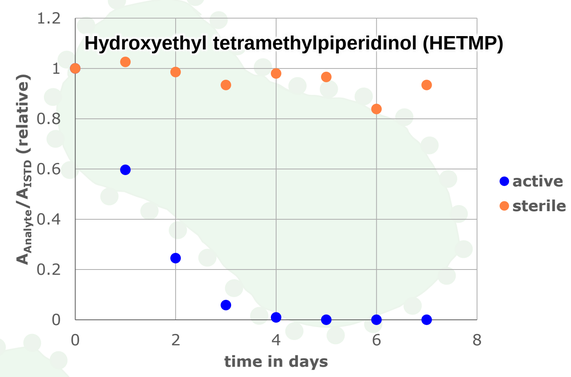
4-MTSC → 4-MTSC TP92

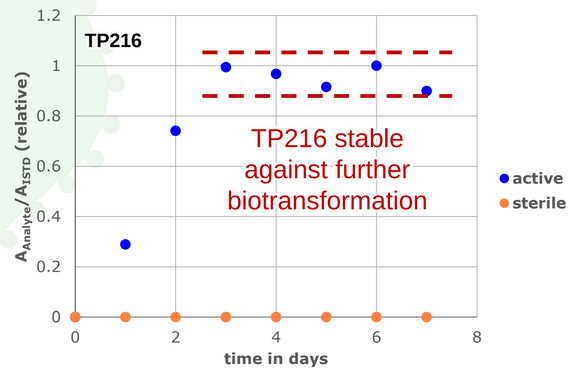




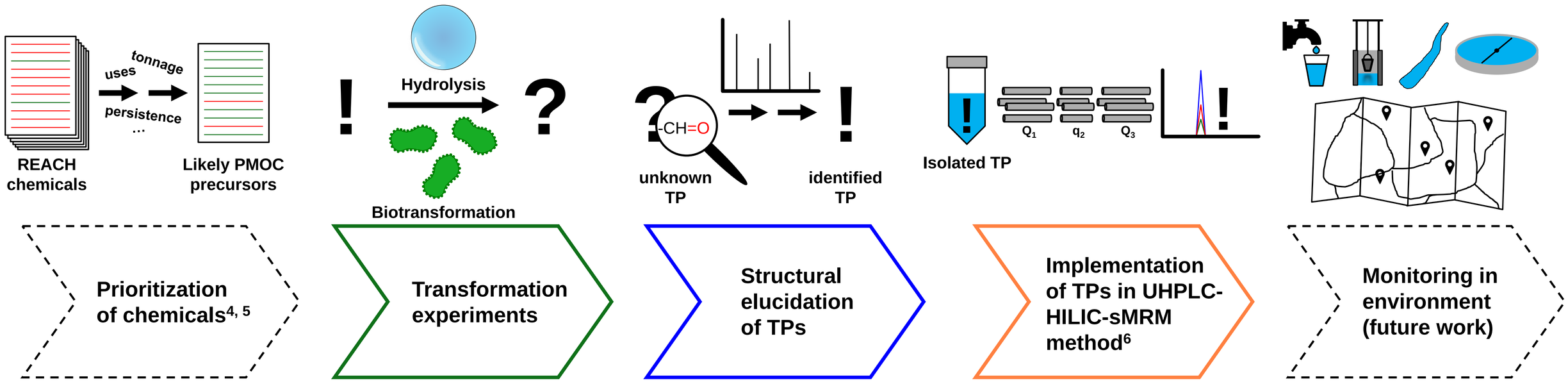
- Hydrolysis of 4-MTSC was investigated
- Hydrolysis procedure adopted from OECD 311 but test period extended to study stability of TPs
- TP92 not stable against further hydrolysis → low priority for monitoring



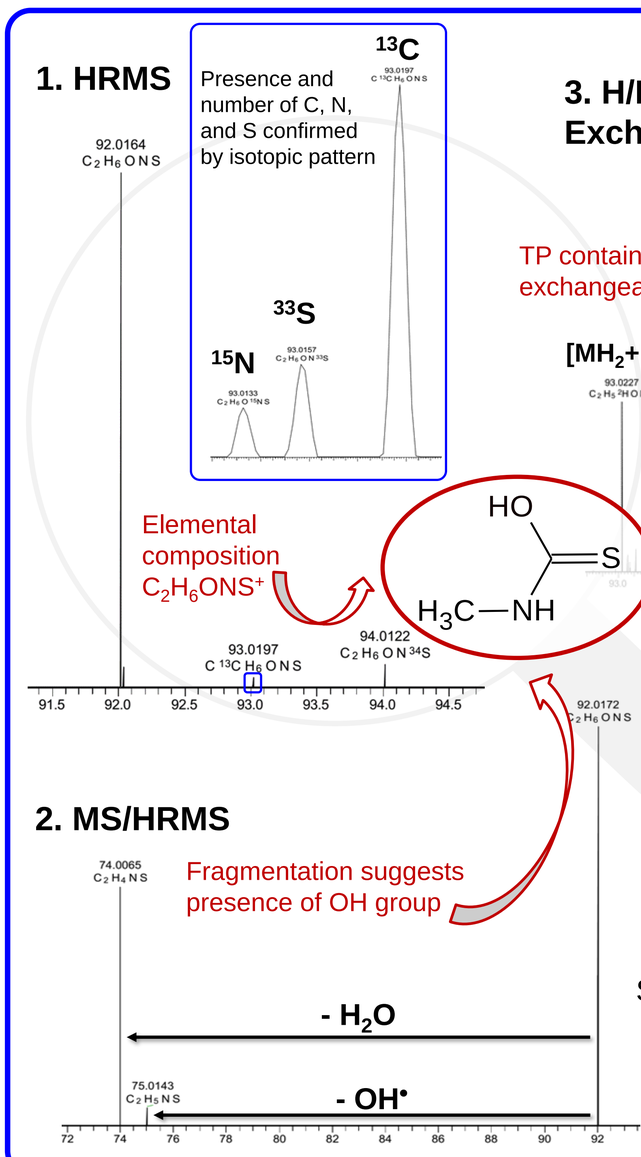




- Biotransformation of HETMP was investigated
- TP216 stable against further biotransformation
  → high priority for monitoring

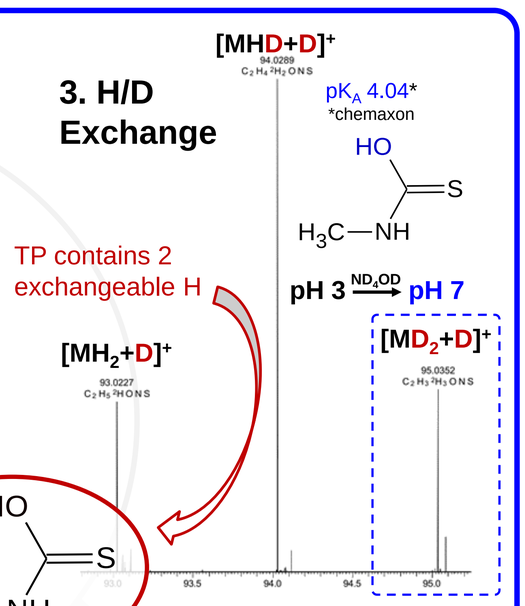


1. HRMS

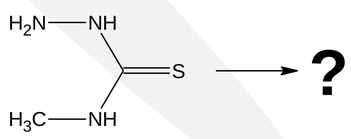


2. MS/HRMS

3. H/D Exchange

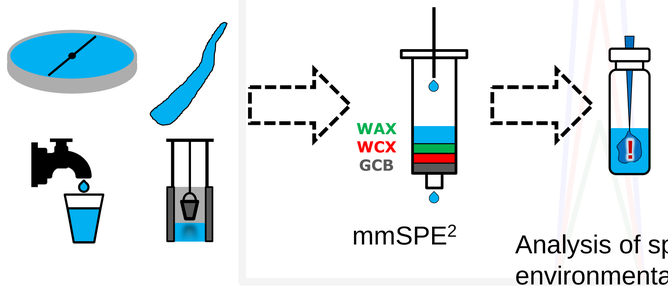


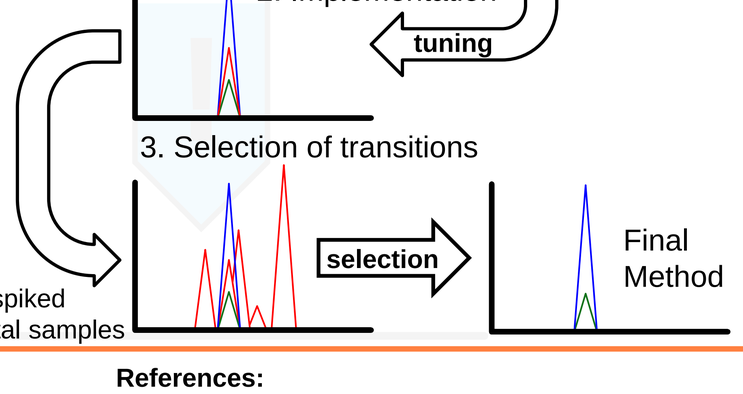
Hydrolysis product of 4-MTSC detected



Structural elucidation with:
HRMS
MS/HRMS
H/D Exchange

- Prioritized TPs were isolated by fractionation with HILIC (if necessary)
- Isolated TPs were included into a UHPLC-HILIC-sMRM method[6]
- Enriched[2] environmental water samples were spiked with isolated TPs and analyzed
- Suitable transitions were selected





Conclusion

- Strategy for TP identification and prioritization shown on two examples
- All in all 15 suspected PMOC precursors investigated, but data evaluation not yet finalized
- Monitoring campaign will allow reliable assessment of environmental relevance

References:
[1] Reemtsma, T., *et al. Environmental Science & Technology* **2016**, *50*, 10308-10315.
[2] Zahn, D., *et al. Water Research* **2016**, *101*, 292-299.
[3] Montes, R. *et al*. *Environmental Science & Technology* **2017,** accepted manuscript
[4] Arp, H. P. *et al*. Environ. Sci. Process Impacts, under revision
[5] Schulze, S. *et al*. in preparation
[6] Zahn, D. *et. al*. in preparation

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