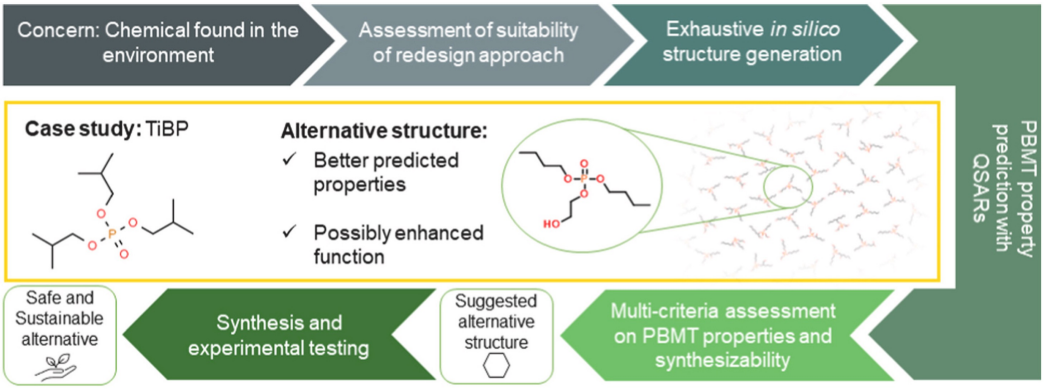
Safe and sustainable by design: A computer-based approach to redesign chemicals for reduced environmental hazards

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Persistency of chemicals in the environment is seen a pressing issue as it results in accumulation of chemicals over time. Persistent chemicals can be an asset in a well-functioning circular economy where products are more durable and can be reused or recycled. This objective can however not always be fulfilled as release of chemicals from products into the environment can be inherently coupled to their use. In these situations, chemicals should be designed for degradation. In this work, a systematic and computer-aided workflow was developed to facilitate the chemical redesign for reduced persistency. The approach includes elements of Essential Use, Alternatives Assessment and Green and Circular Chemistry and ties into goals recently formulated in the context of the EU Green Deal. The organophosphate chemical triisobutylphosphate (TiBP) was used as a case study for exploration of the approach, as its emission to the environment was expected to be inevitable when used as a flame retardant. Over 6.3 million alternative structures were created in silico and filtered based on QSAR outputs to remove potentially non-readily biodegradable structures. With a multi-criteria analysis based on predicted properties and synthesizability a top 500 of most desirable structures was identified. The target structure (di-n-butyl (2-hydroxyethyl) phosphate) was manually selected and synthesized. The approach can be expanded and further verified to reach its full potential in the mitigation of chemical pollution and to help enable a safe circular economy.



Systematic, computer-aided approach to redesign for less persistent chemicals

[1] van Dijk, J., Flerlage, H., Beijer, S., Slootweg, J. C., & van Wezel, A. P. (2022). Chemosphere, 296, 134050.