

Student Research

SR 2022.003

*In silico* tools to prioritize transformation products of active substances originating during drinking water treatments: S-metolachlor as a proof of principle.

8 December 2022

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Surface water and groundwater used as drinking water sources can be contaminated at low levels with different active substances from plant protection products. When drinking water treatments are applied, these active substances can be transformed into new products called transformation products (TPs). Predicting the formation of TPs and potential health hazards is pivotal to assessing the risks of these specific contaminants in drinking water sources and decision-making on mitigation actions through water sources protection and water treatment processes. The student research project (Dec 2021 - Nov 2022) focused on selecting freely available *in silico* tools to predict the formation of TPs in drinking water treatment processes and

their health hazards to prioritize further research. The prioritization scheme was applied to S-metolachlor, a widely used herbicide in Europe. S-metolachlor TPs were predicted and prioritized based on qualitative hazard assessment using selected freely available *in silico* tools. This research addressed the effectiveness of *in silico* tools in predicting, prioritizing, and evaluating TPs and pointed out the necessity of further research and software development. Lastly, this research tentatively identified some of the prioritized S-metolachlor TPs in water samples treated with rapid sand filtration (Brunner et al., Chemosphere, 2019). Follow-up research is recommended to focus on the refinement, validation and implementation of the applied prioritization scheme.

See also:

<https://library.kwrwater.nl/publication/68647337/>

<https://library.kwrwater.nl/publication/69204342/>

More information:

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Keywords: *in silico* tools, transformation products, drinking water treatments, predictive toxicology