AMSTERDAM INTERNATIONAL WATER WEEK

Abstract Title	Prediction of organic micropollutant removal in drinking water treatment processes, based on QSPR modelling
Topic	x Improving water quality O Resilient water systems O Circular solutions: Reuse, Recover and Recycle O Transitions in water, agro/food and energy
Challenges and Solutions	1. Smart water solutions (digital)
Author(s), highlight corresponding author	1.Martin Korevaar, KWR Water Research Institute, The Netherlands 2. Bas Wols, KWR Water Research Institute, The Netherlands 3. Emile Cornelissen, KWR Water Research Institute, The Netherlands; University of Ghent, Belgium 4. Roberta Hofman-Caris, KWR Water Research Institute, The Netherlands; Utrecht University of Applied Sciences, The Netherlands; Wageningen University and Research, The Netherlands
Abstract	In sources for drinking water more and more organic micropollutants (OMPs) are being detected. In principle different technologies (membrane filtration, adsorption onto activated carbon and (advanced) oxidation processes) can be applied to remove these OMPs, but it is expensive and time consuming to test these technologies for ever newly detected OMP. For that reason models have been developed, which can be used to predict which treatment technique may be most effective. Data were collected from pilot experiments conducted over the past decade at KWR and from literature. Depending on the process, OMP specific information originating from 100-500 compounds was used to train models. For these compounds Quantitative Structure Property Relationships (QSPRs) were developed, to find a statistic relation between e.g. reaction

parameters (like quantum yield, and reaction constants) and the molecular structure. These compound specific parameters were used in process models to predict the OMP removal by advanced oxidation, membrane filtration and activated carbon filtration (Figure 1).

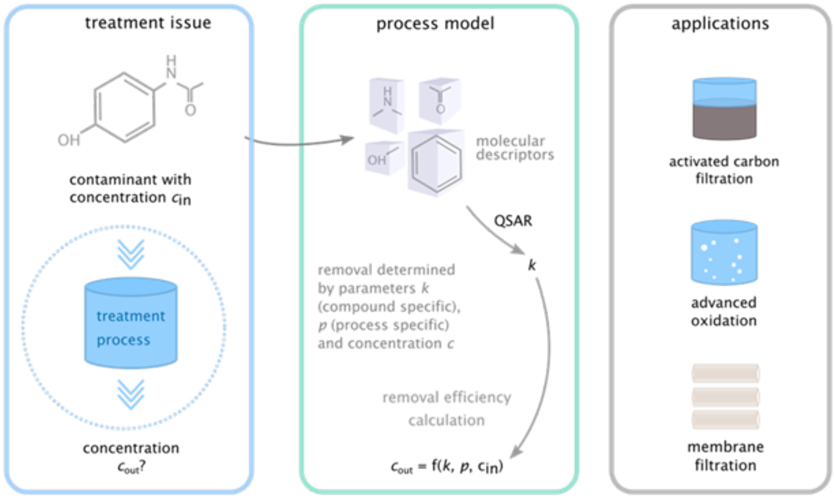

Figure 1: OMP removal predictions using process models and statistical models (QSAR/QSPRs).

For validation purposes, a representative selection of OMPs was made. For this purpose a mathematical selection method has been applied, resulting in a set of 30 different OMPs. These 30 OMPs were tested in pilot installations for the three treatment techniques..

For oxidation, process models combined with QSPRs for OMP specific kinetic parameters (OH• radical and O_3 reaction rate constants, quantum yield) resulted in models that can predict the oxidation and/or photolysis of OMPs in UV, O_3, O_3/H_2O_2, UV/H_2O_2, and UV/O_3 processes. Compared to the measured set of 30 OMPs, an accuracy of ≥ 80 % was achieved. Furthermore, models were developed to predict the removal of OMPs by means of spiral wound nanofiltration (NF) and reverse osmosis (RO) membranes and capillary NF membranes. QSPRs were used to predict the permeability of the membranes (Figure 2). An accuracy of ≥ 80 % can be achieved in this way.

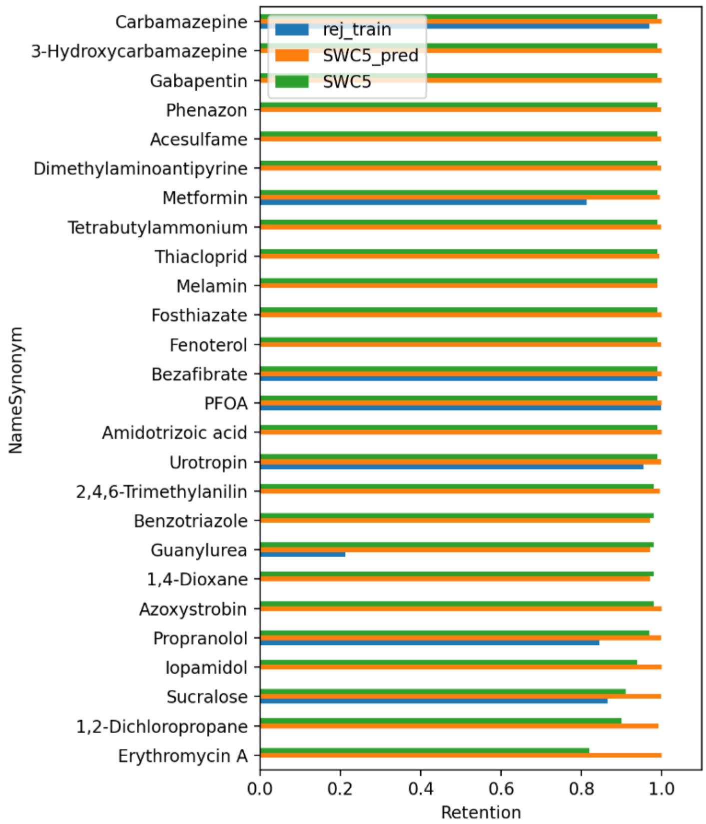

Figure 2: OMP removal from drinking water by means of RO. Orange predicted removal, green measured removal, blue average removal by means of other types of membranes.

Finally, a model has been developed to predict breakthrough of OMPs on granular activated carbon filters. In pure water, without NOM, this breakthrough can accurately be predicted, but in NOM containing water NOM competition and pore blocking have to be taken into account. By describing NOM as an equivalent background component (EBC) the effects can only partly be accounted for. At the moment, this EBC model is being improved to account for the effects of different NOM fractions onto the adsorption behavior of different types of OMPs.

The resulting models provide an efficient method to predict which type of removal technology may be applicable for a new type of OMP. The models have been incorporated into an online tool: AquaPriori, which allows water industry to make a quick evaluation of the removal of an OMP. Naturally, the predictions still will have to be experimentally checked, but the experiments can be made far more effective, which will safe time and costs.

Figures/diagrams/illustrations	Up to 2 (in abstract)