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Activity-based fate modelling for risk assessment of three ionizable organic compounds (triclosan, furosemide, ciprofloxacin)

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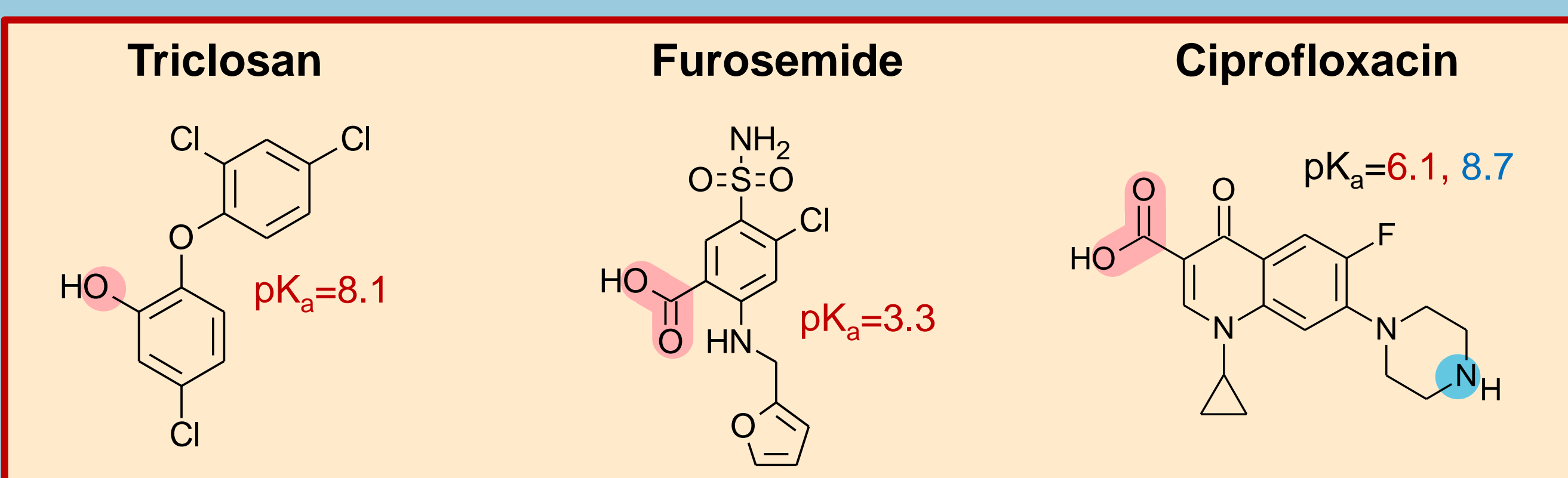
Background and target substances

Most pharmaceuticals are ionizable compounds

Ionizable chemicals are 49% of all substances registered according to the REACH protocols [1]. 77.5% of pharmaceuticals assessed within a data set of over 500 substances were found to ionize at biologically relevant pH range [2].

Prediction of the fate of ionizable chemicals: a novel approach

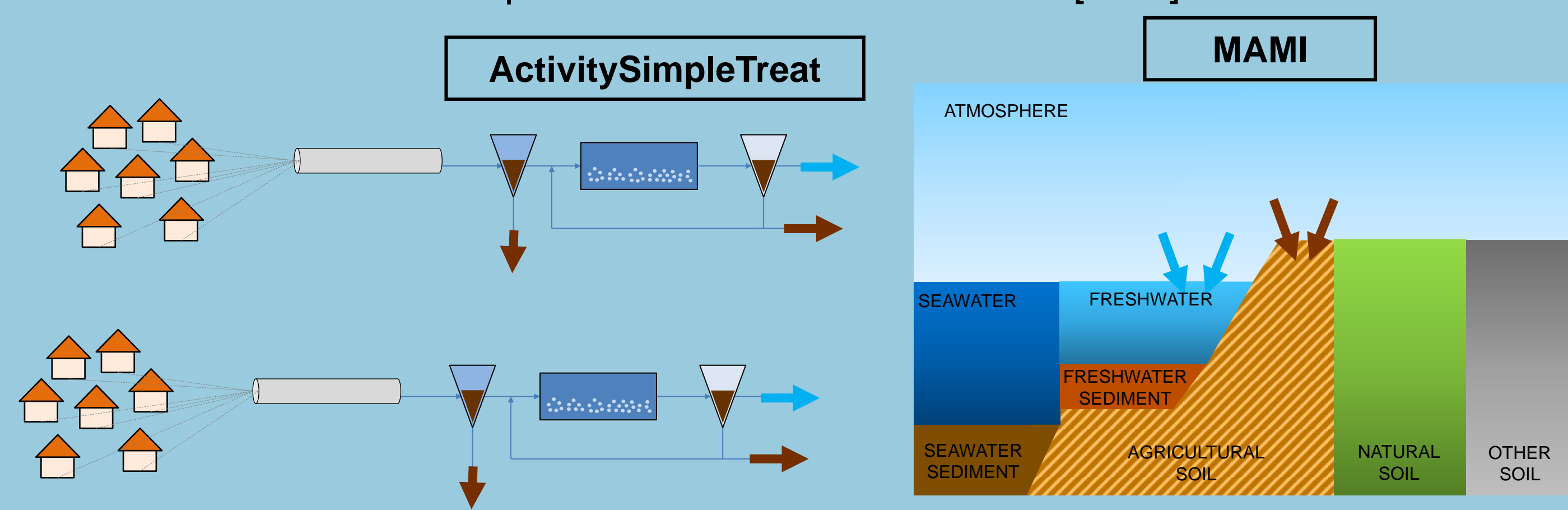
Activity-based models have been developed to predict the environmental fate of organic ionizable compounds, based on their QSAR properties [3,4].



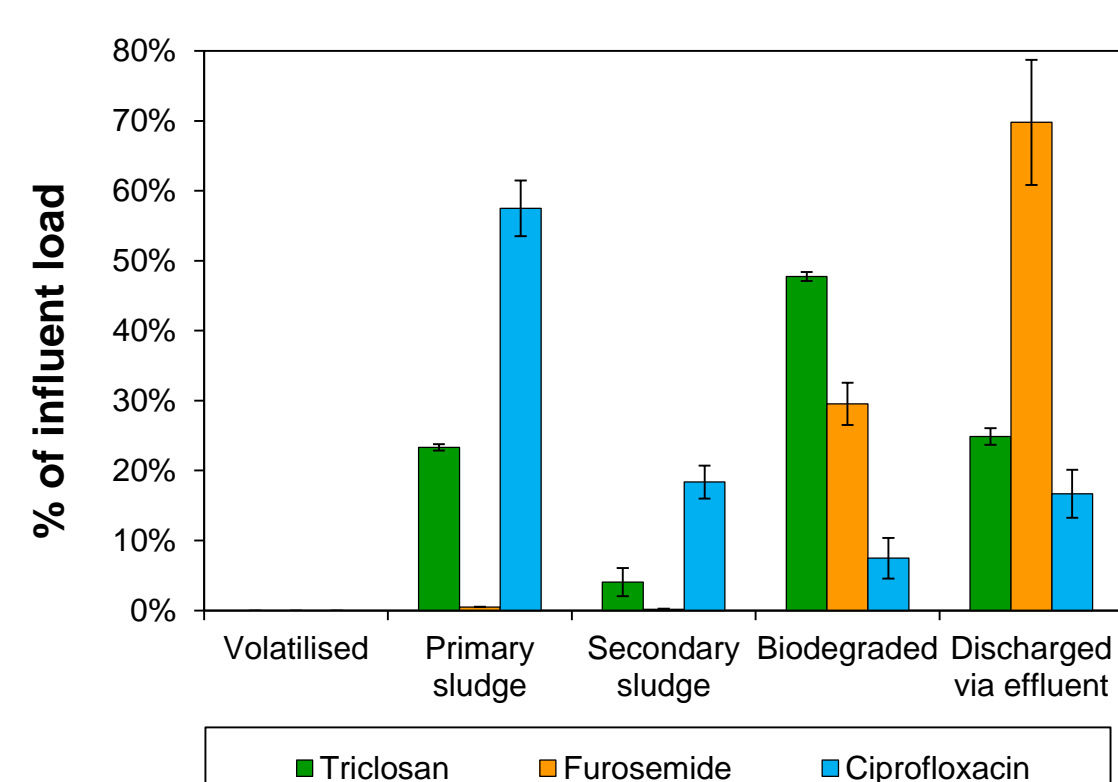
Objectives and Methods

Environmental risk assessment of three ionizable pharmaceuticals

- Prediction of fate according to REACH regulation: local (C_{local}) and regional concentrations ($PEC_{regional}$) of parent substances
- Combination of steady-state models for WWTP fate (Activity SimpleTreat) and regional fate (MAMI-Multimedia Activity Model for Ionics) [3,4]
- Assessment of real emission scenarios (annual average): Lower Saxony, Southern Sweden, Denmark, Northern Italy
- Validation of model predictions with literature data [5-12]

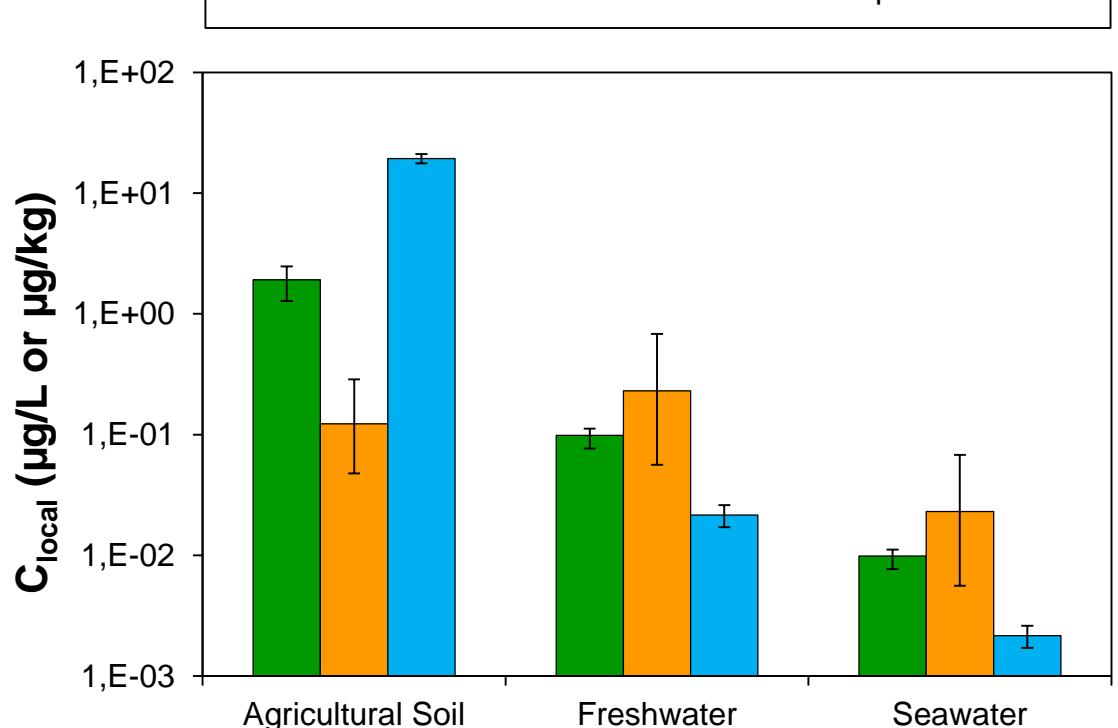


Model predictions



WWTP fate predictions

- Furosemide had the lowest removal (> 70% discharged via effluent).
- Triclosan was ~50% biodegraded and 25% discharged via effluent.
- Ciprofloxacin was mostly removed in the sludge (>70%) due to very high sorption coefficient.

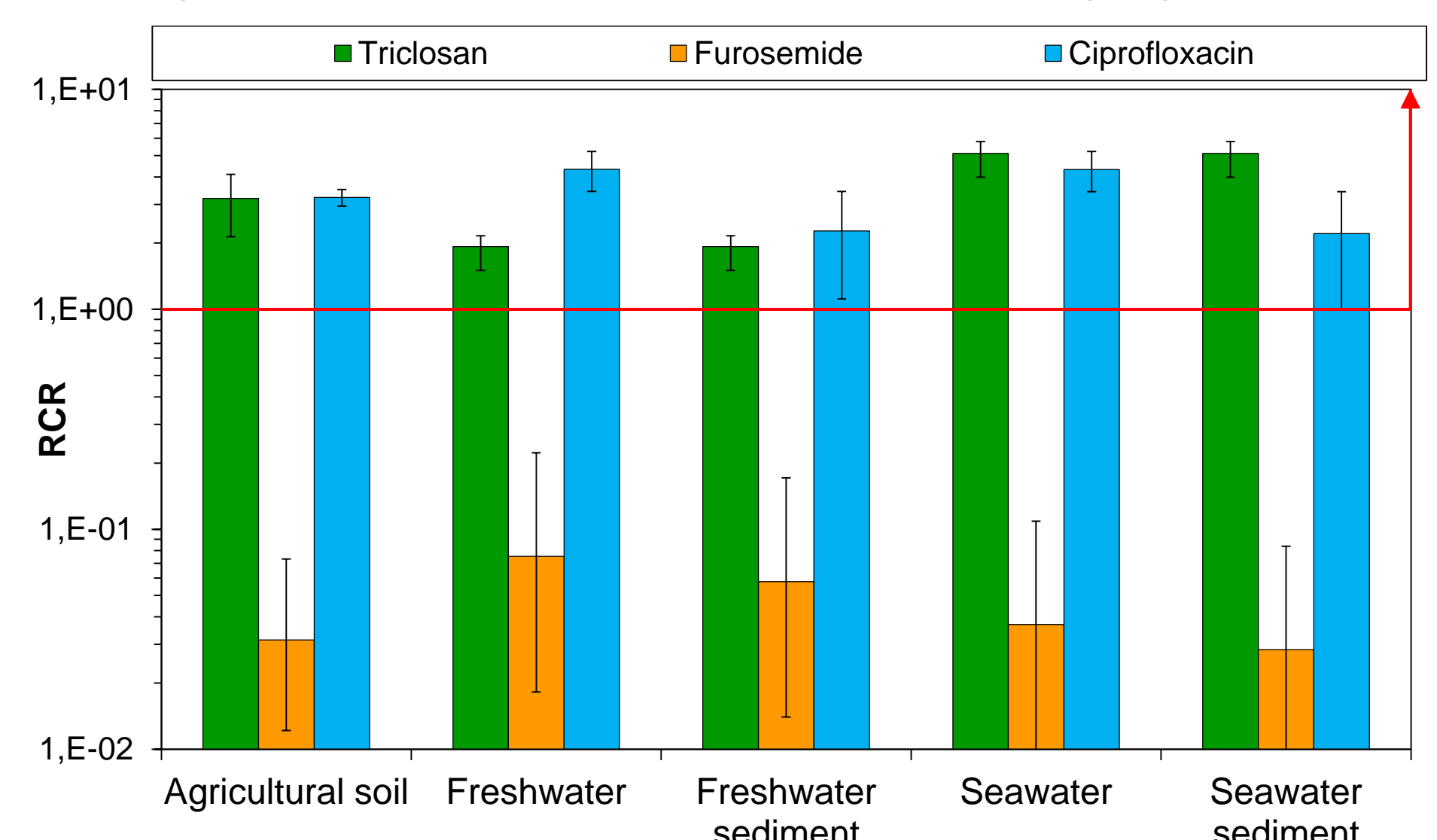


C_{local} in receiving freshwater bodies were estimated to be $\geq 0.1 \mu\text{g/L}$ for triclosan and ciprofloxacin. Ciprofloxacin was also found to accumulate in soil ($C_{local} > 10 \mu\text{g/kg}$), as a result of sludge amendment.

$PEC_{regional}$ estimated with MAMI were found to be < 6% of C_{local} (not shown).

Risk characterization

PEC_{local} (by combining C_{local} and $PEC_{regional}$) were used to calculate Risk Characterization Ratios (RCRs). Predicted Non-Effect Concentrations (PNECs) were defined from worst cases in literature or calculated according to REACH TGD. PNECs used were 53 ng/L (triclosan), 3.1 $\mu\text{g/L}$ (furosemide), 5 ng/L (ciprofloxacin) in water and 0.6 $\mu\text{g/kg}$ (triclosan) in soil.



$$RCR = \frac{PEC_{local}}{PNEC}$$

$RCR > 1$ was found for triclosan (1.9–5.1) and ciprofloxacin (2.2–4.3). No potential risk was exhibited to furosemide ($RCR < 0.2$).

Validation

Results were compared with WWTP removal rates and concentrations in literature to test the reliability of the models.

Substance	WWTP removal			Concentrations in freshwater			
	Simulated	Literature	Ref.	Scenario	PEC_{local}	Literature	Ref.
Triclosan	74%–76% (46–48% degraded)	55%–98% (48% degraded)	[5,6]	Lower Saxony	80 ng/L	3–90 ng/L	[9,10]
Furosemide	21%–33%	21%	[7]	Denmark	680 ng/L	250–420 ng/L	[11]
Ciprofloxacin	80%–87% (70%–82% in sludge)	88% (83% in sludge)	[8]	Northern Italy	17–26 ng/L	14–26 ng/L	[12]

Conclusions

- The modification of the standard fate models (SimpleTreat and Level III regional model) to multispecies models for ionizable compounds was possible and allowed prediction of acids' and zwitterions' fate.
- Model predictions of WWTP fate and of local concentrations were realistic.
- Potentially high risk at local level was associated to triclosan and ciprofloxacin in water, sediment and soil compartments in all scenarios assessed.
- Further investigation is needed, as fate is influenced by e.g., temporal variations of emissions and conjugates' retransformation [13,14].

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In all the graphs presented, columns represent the mean value (of % of influent load, C_{local} and RCR) among all scenarios considered, and error bars refer to the range in which those values are included.

