Environmental and Spatial Drivers Explain Variability of Contaminants of Emerging Concern

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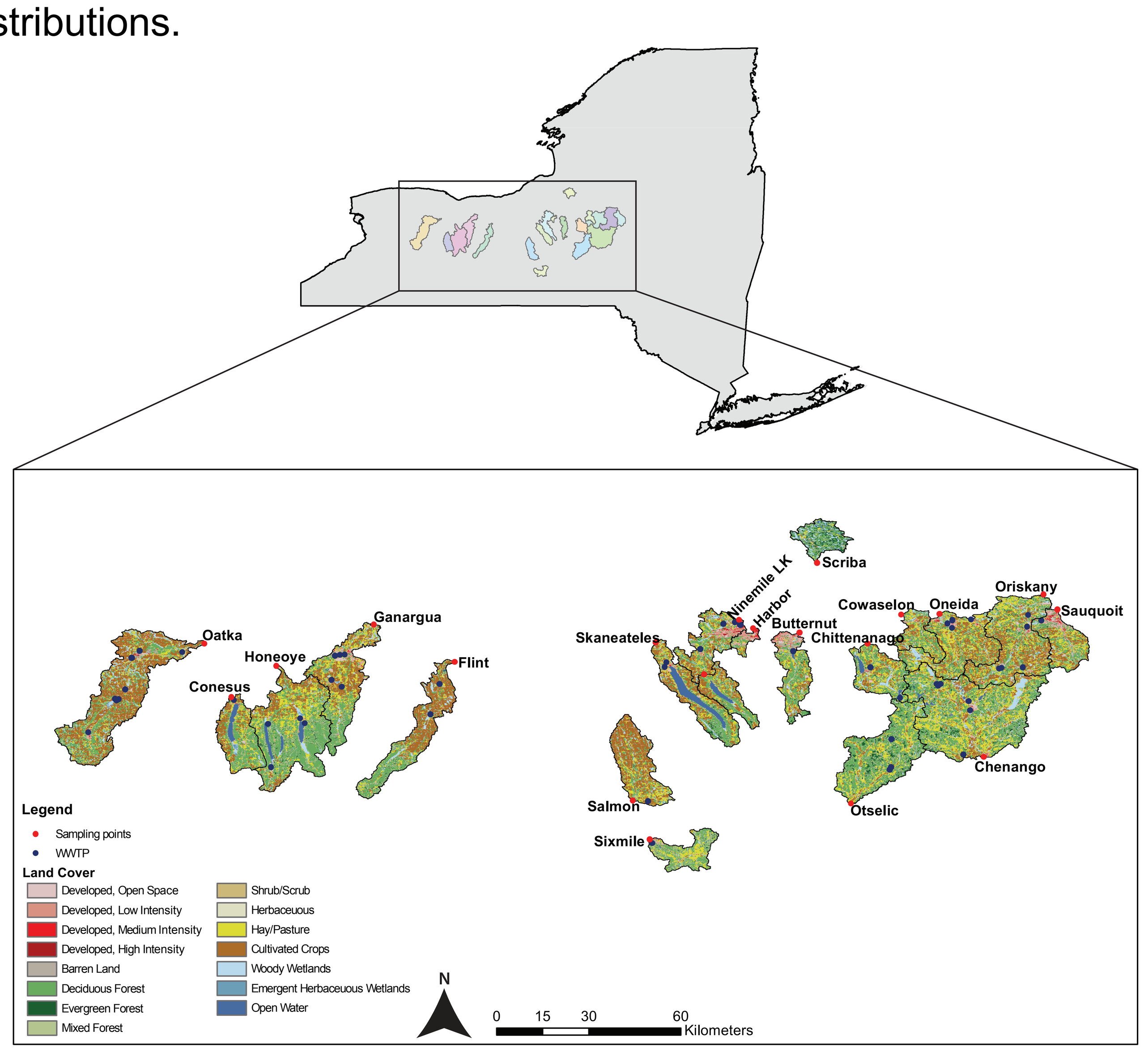
Research Objectives

Monitoring studies have identified the occurrence of hundreds of contaminants (CECs) throughout the environment. The presence of CECs is often associated with degraded water quality, which can be harmful to ecosystems as well as human health. Despite their ubiquitous presence, relatively few studies explore how watershed characteristics, land use, and hydrological processes affect CEC occurrence, which obscures our understanding of spatio-temporal influences and the ultimate fate of these chemicals in surface water. Our research questions were:

- Which climate and hydrologic processes influence CEC dynamics in surface water?
- How does land cover impact detected number of CECs as well as their concentrations?

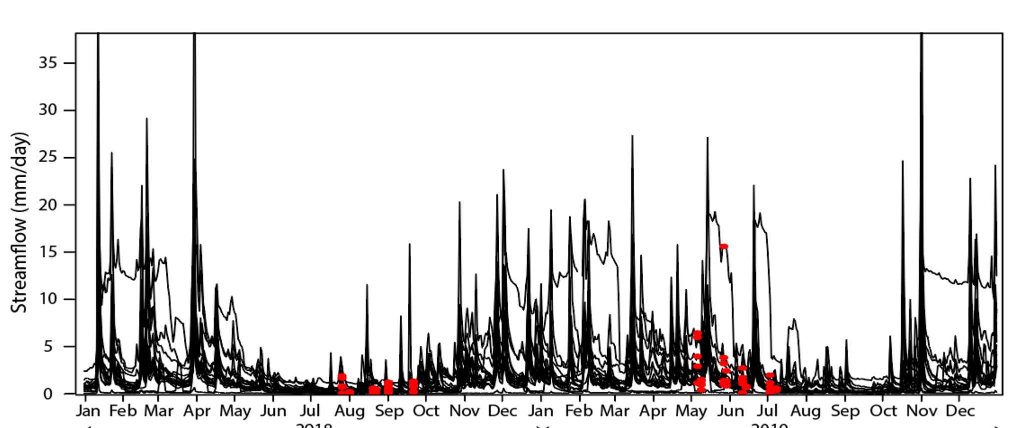
Study Area

We performed water quality sampling at regional scales to study hydroclimatological and watershed use influences on observed CEC dynamics across 20 watersheds in central NY with varying land cover distributions.



Sampling

To establish spatio-temporal CEC patterns, grab samples were collected during two rounds of sampling across variable hydrologic conditions. Samples were taken 20 to 25 days apart during late summer – early fall in 2018 and late spring – early summer in 2019.

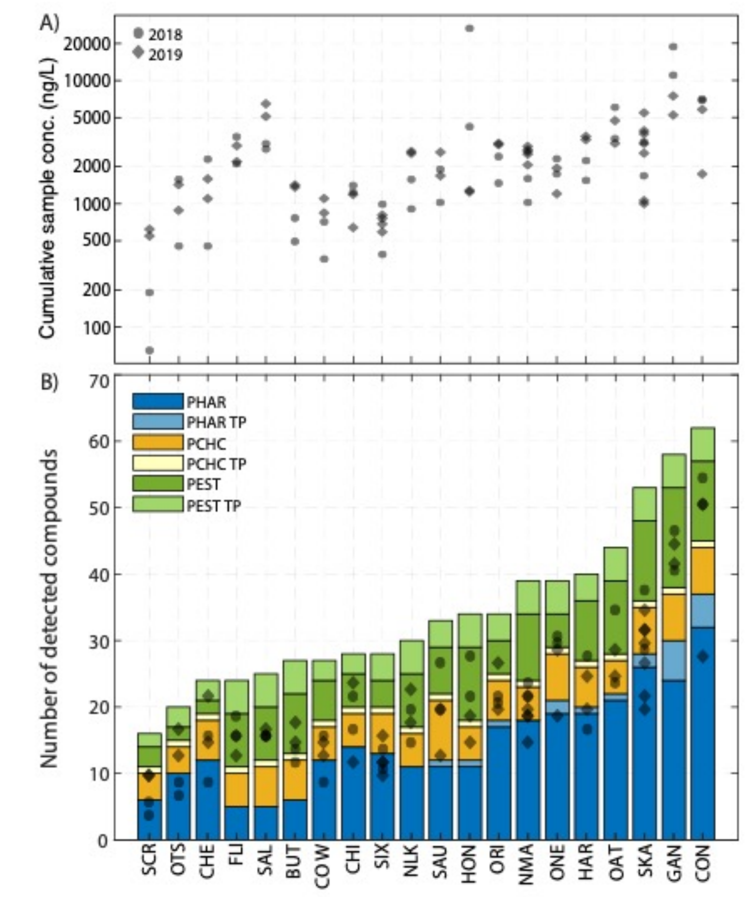


2018 sampling period was much drier compared to 2019 sampling period.

CEC Variability in Time and Space

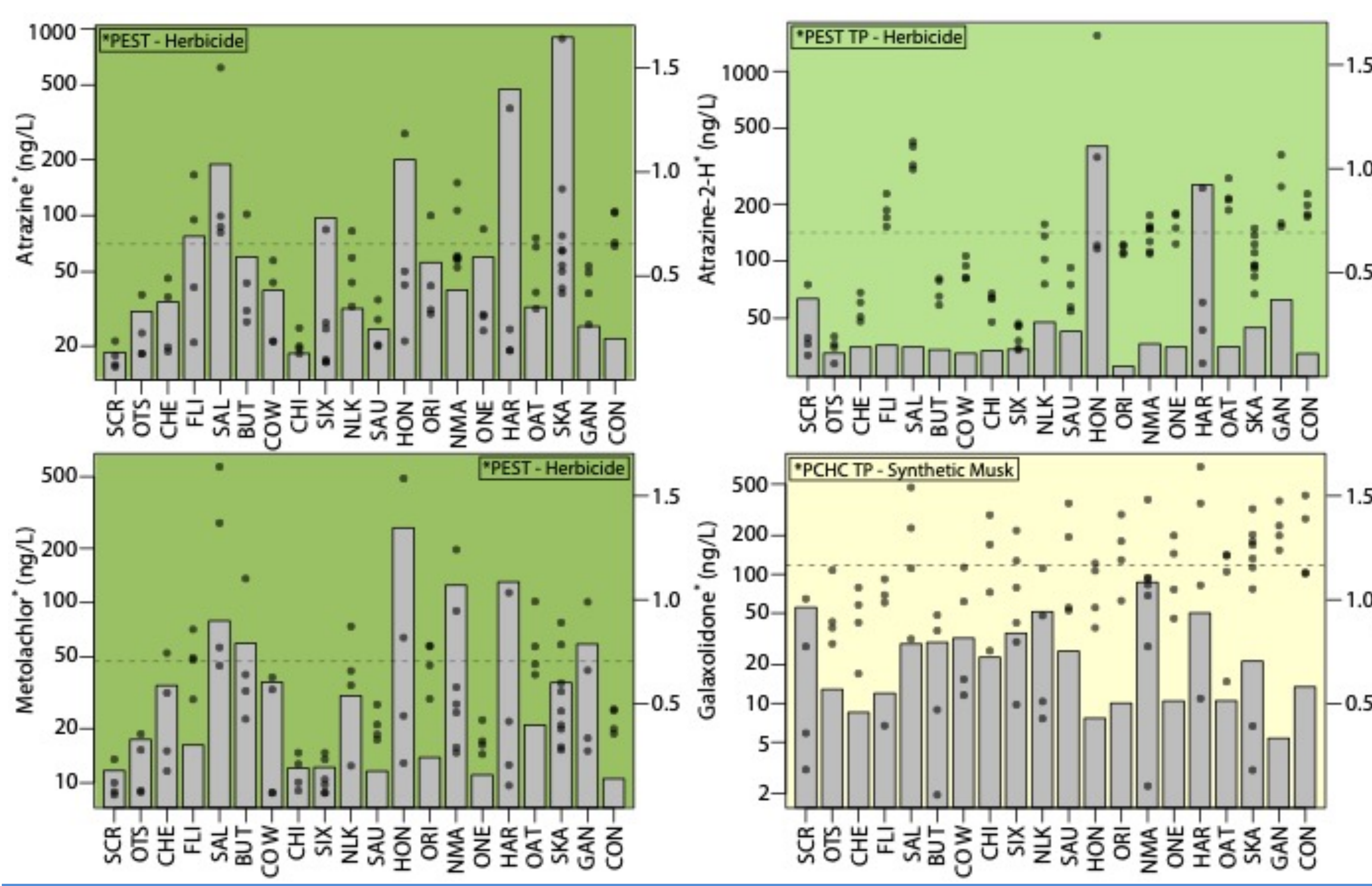
Samples were analyzed using liquid chromatography - high resolution mass spectrometry (LC-HRMS) and screened for 344 CECs (including transformation products [TP]) using a target suspect database. Overall, 79 compounds were identified:

- 38 Pharmaceuticals (PHAR) and 6 PHAR TP
- 9 Personal Care Products (PCHC) and 1 PCHC TP
- 20 Pesticides (PEST) and 5 PEST TP



Total number of detected CECs varied from site to site, ranging from 18 (SCR) to 62 (CON). Cumulative sample concentrations varied in time as well as among study sites; however, highest detected number of CECs did not correlate well with largest cumulative sample concentrations.

Four of the detected compounds were found in all samples: atrazine, atrazine-2-H, metolachlor, galaxolidone. CEC concentrations varied greatly among study sites, but variation in time ranged from compound to compound.



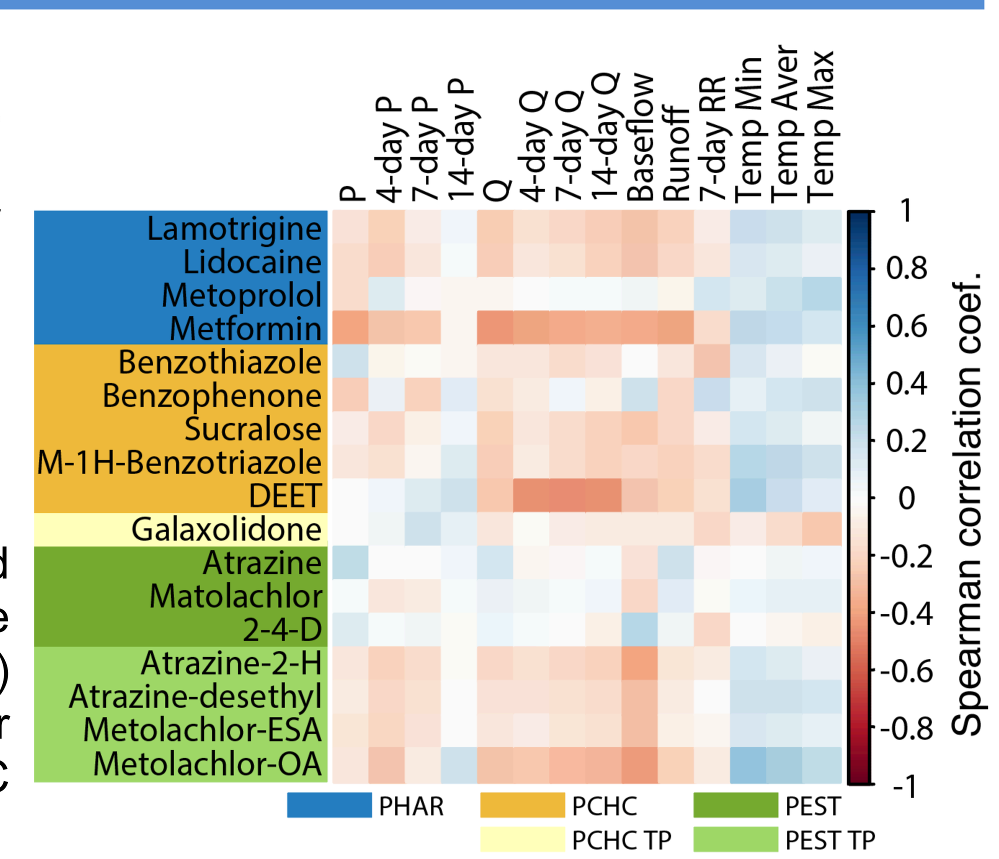
Atrazine-2-H: Highly variable in space, but varied minimally in time.

Galaxolidone: Highly variable in space and time.

Environmental Influence

The influence of environmental variables on observed concentrations varied across compounds. Precipitation and streamflow were negatively correlated with most PHAR, PCHC, and PEST TP compounds, suggesting that dilution plays an important role in CEC dynamics.

Some compounds (e.g. DEET) showed high correlation with long term climate variables (4-day, 7-day, and 14-day Q) highlighting the influence of prior hydrologic conditions on CEC dynamics.



Land Cover Impact

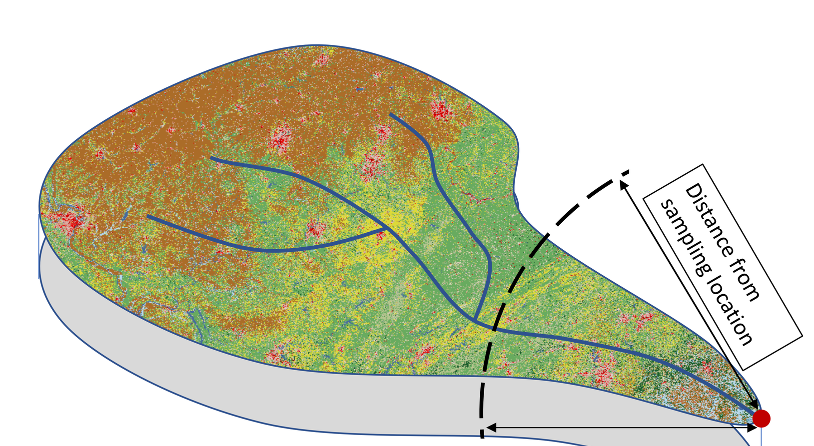
Spatial analysis is useful in evaluating non-point sources of CECs, with land cover (e.g. agricultural and urban land cover) being a proxy for CEC sources. We used the percentage of agricultural and urban land cover at various spatial scales as predictor variables to estimate total number of detected CECs as well as their detected concentrations.

- *Predicting Total Number of Detected CECs by Type*

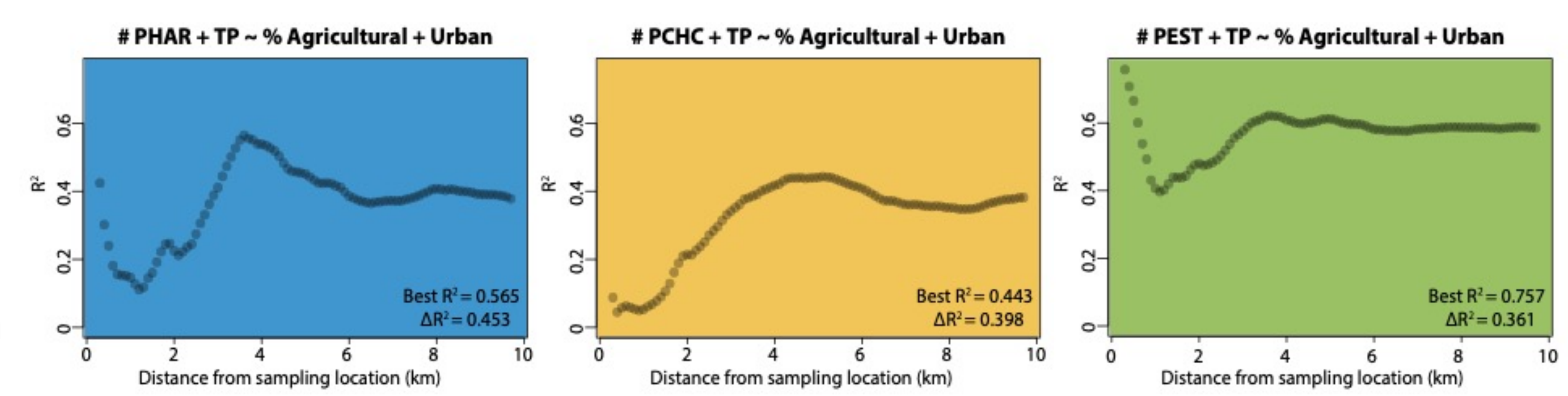
Ordinary Least Square (OLS) modeling was used to predict the presence of CECs across three CEC types: PHAR, PCHC, PEST. First, we used watershed scale land cover percentages to predict total number of detected CECs. Model results reported as r^2 were as follows:

Land cover (%)	PHAR	PHAR TP	PHAR + TP	PCHC	PCHC + TP	PEST	PEST TP	PEST + TP
% Agricultural	0.005	0.016	0.007	0.017	0.017	0.190	0.370	0.243
% Urban	0.010	0.001	0.008	0.070	0.070	0.024	0.002	0.019
% Agricultural + Urban	0.019	0.020	0.019	0.110	0.110	0.261	0.406	0.311

Distance weighting model



OLS models were created using agricultural and urban land cover percentages as predictor variables at increasing distance from each sampling location to evaluate if proximity to outlet has any effect on predicting total number of PHAR, PCHC, and PEST. Results show that model accuracy increased with proximity to the sampling location, reaching *r^2 = 0.76 for PEST + TP detections.*



- *Predicting CEC Concentrations*

OLS modeling was also used to analyze relationships between watershed land cover and compound concentrations. Models for six CECs produced *r^2 > 0.3.* Results show that our ability to predict CEC concentrations increased with distance from sampling site, reaching *r^2 = 0.62* for persistent compounds like atrazine transformation products.