



IAWWTF

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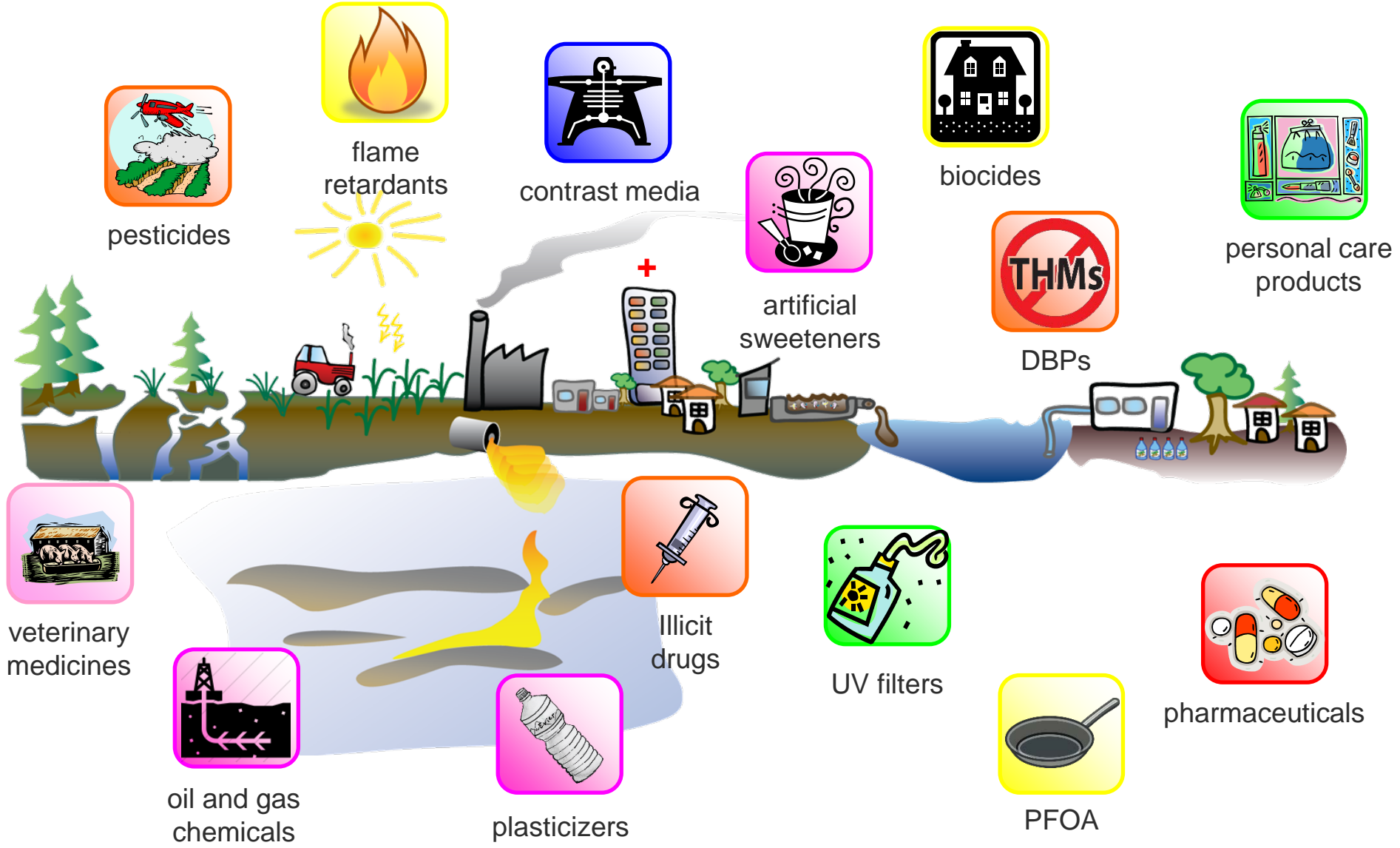
Damian E. Helbling, Assistant Professor, Civil and Environmental Engineering, Cornell University

Emerging Water Quality Concerns: Pharmaceuticals & Microplastics



Tompkins County
Environmental Management Council
8 December 2016

Other emerging chemicals in urban water systems

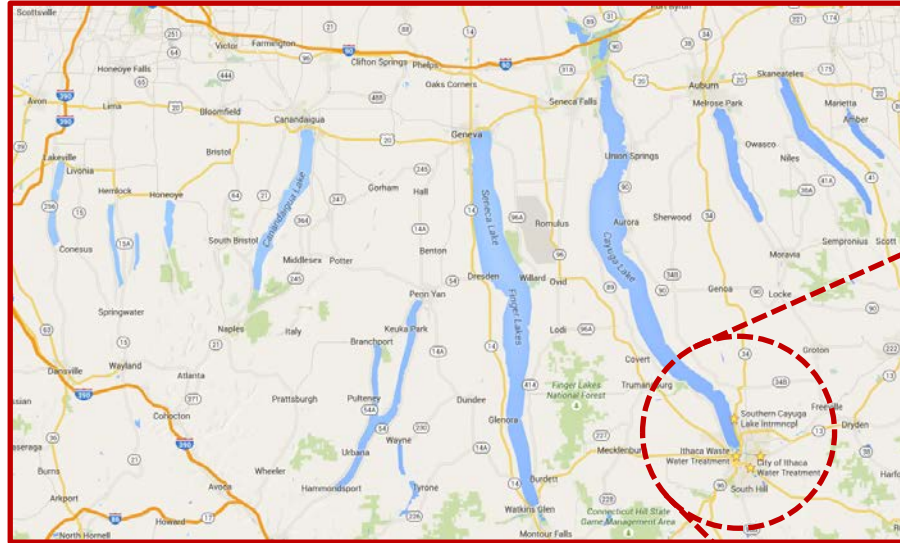


One central question of research in the Helbling group

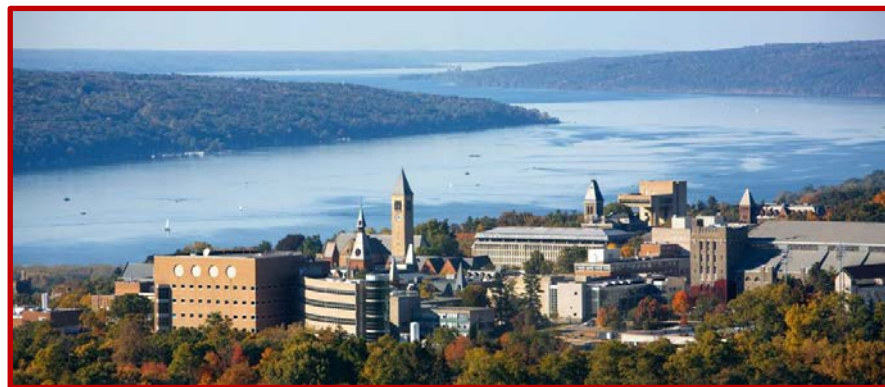
*How can we be more **comprehensive** in our monitoring for **emerging chemical contaminants**?*



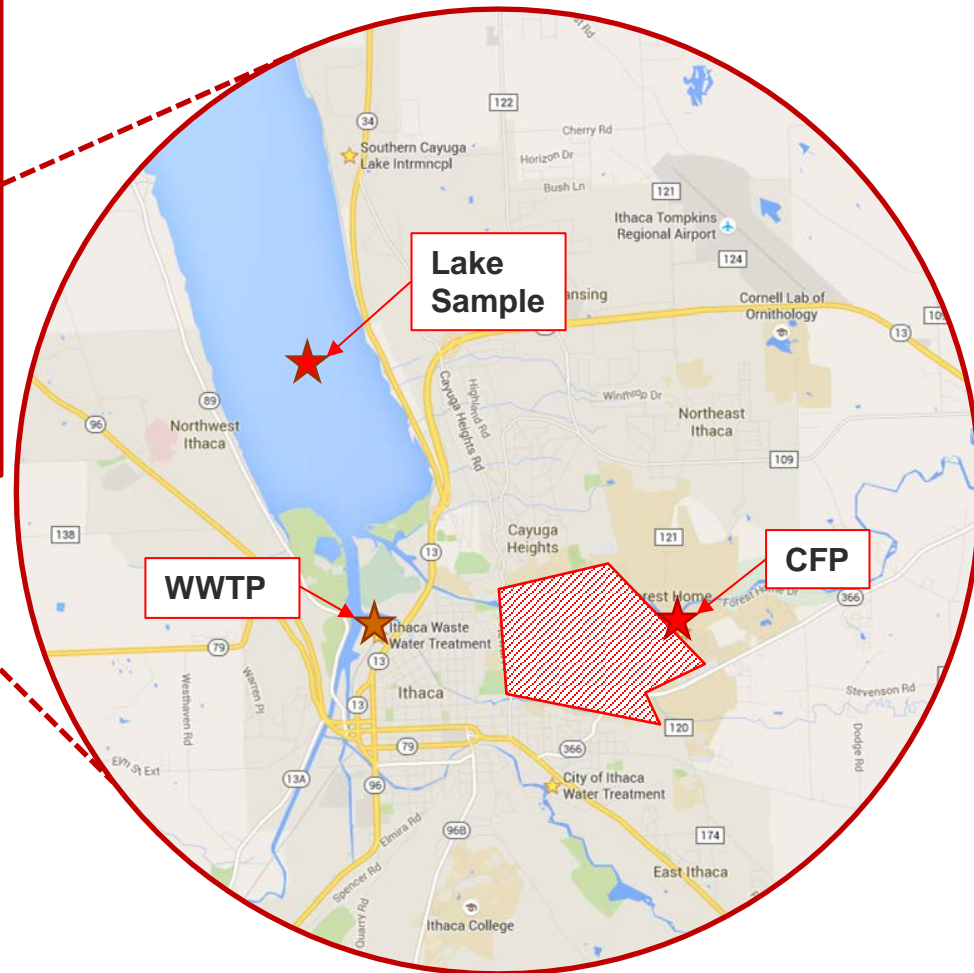
Suspect screening in the Ithaca urban water system



Finger Lakes region, Upstate New York
Source: Google Maps



Source: cornell.edu

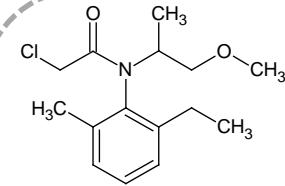
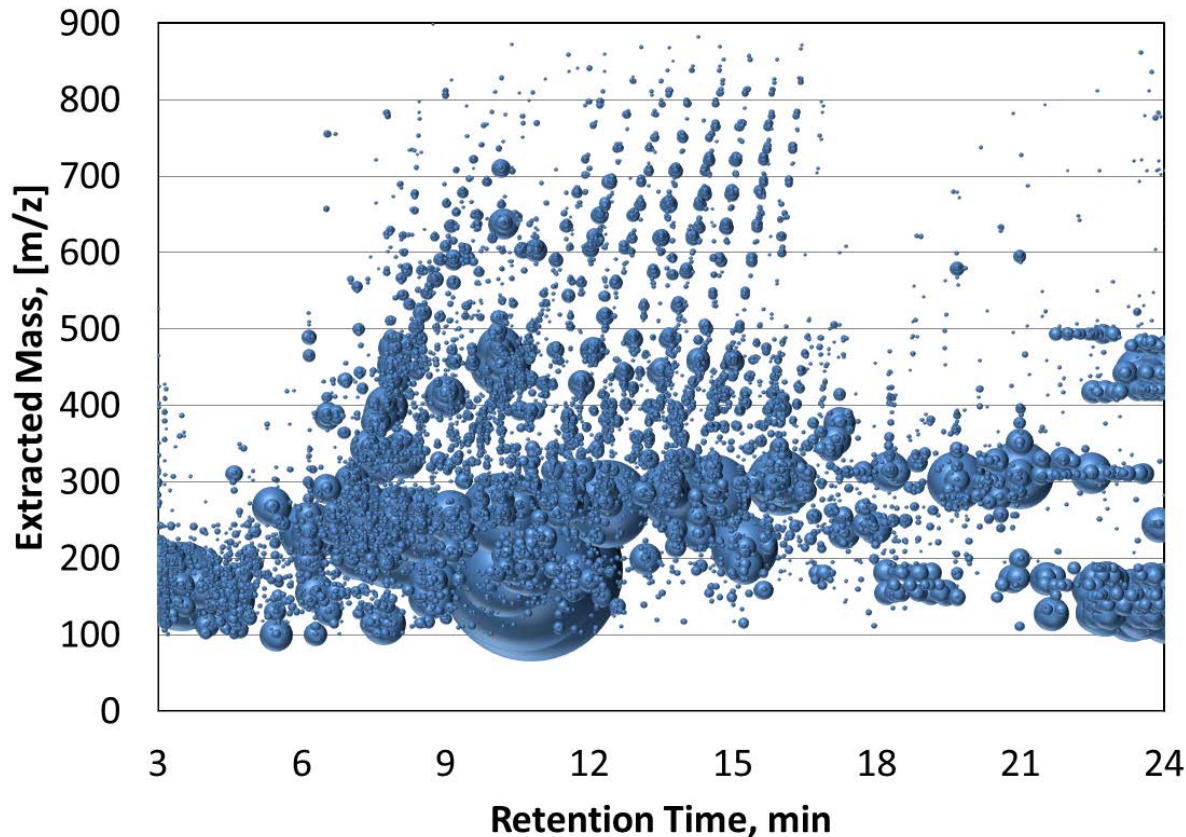


Suspect screening in the Ithaca urban water system

1,113

Pesticides, pharmaceuticals, personal care products, industrial chemicals...

Full-scan high-resolution MS acquisition



metolachlor

$C_{15} H_{22} Cl N O_2$

$[M+H]^+$ 283.1339

Expected isotope (MS) pattern::

$[M+H+1]^+$ 284.1367 (15%)

$[M+H+2]^+$ 285.1304 (32%)

$[M+H+3]^+$ 286.1338 (5%)

Predicted Retention Time: 10.5 min

Predicted MS2 fragments:

252.11

176.14

134.10

146.10

254.11

Suspect screening – application

Environmental
Science
Water Research & Technology



PAPER

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Cite this: DOI: 10.1039/c6ew00248j

Emerging investigators series: prioritization of suspect hits in a sensitive suspect screening workflow for comprehensive micropollutant characterization in environmental samples†

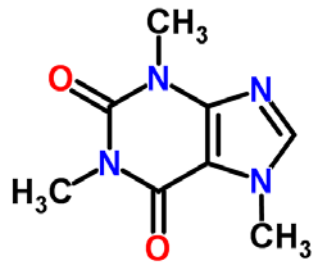
Amy L. Pochodylo and Damian E. Helbling*

The emergence of suspect screening has enabled the comprehensive characterization of micropollutants in water systems. In this work, we developed a sensitive suspect screening workflow and applied it to characterize the occurrence of micropollutants in eighteen water samples collected from an urban water system in New York State. We used high-resolution mass spectrometry to generate high-resolution mass spectra from the water samples and compile 1113 chemical substances including pesticides, pharmaceuticals, personal care products, and other chemicals. The suspect screening workflow included peak picking, pattern scoring, a replication filter, blank subtraction and artifact removal. Each step in the workflow relied only on the quality of the analytical data. We used a set of compounds that covered a broad range of physicochemical properties to optimize the suspect screening workflow to the data acquired from the vials. We evaluated different prioritization strategies that ranked the resulting suspect hits according to their predicted toxicity and persistence in the environment.

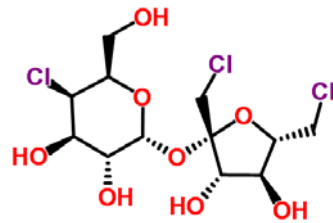
Acknowledgements

We thank Patrick Phillips (USGS) and Tia-Marie Scott (USGS) for coordinating the sampling campaign. We thank Jose Lozano, Chris Bordlemay, and Susan Allen-Gil for useful discussions. This work was supported by the College of Engineering and the School of Civil and Environmental Engineering at Cornell University. A. L. P. acknowledges NSF GRFP grant no. 1144153.

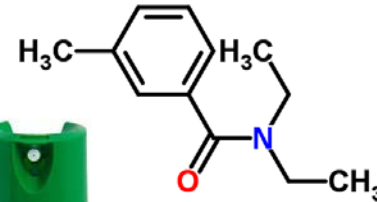
Suspect screening – application



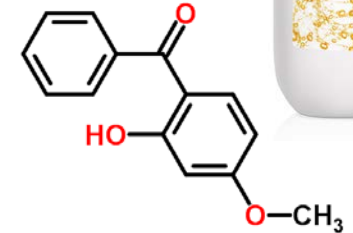
caffeine



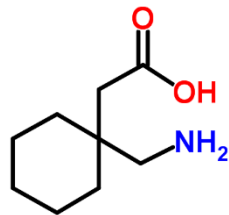
sucralose



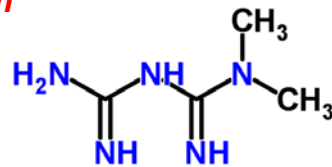
DEET



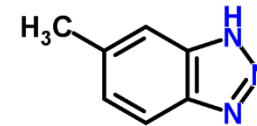
benzophenone-3



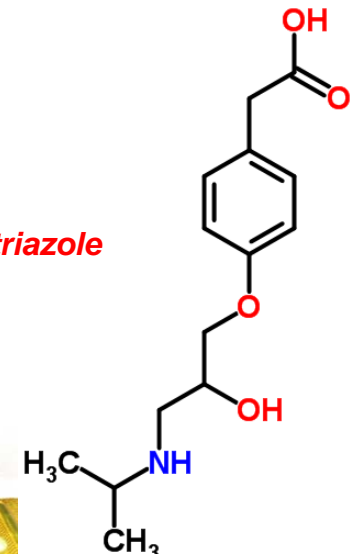
gabapentin



metformin

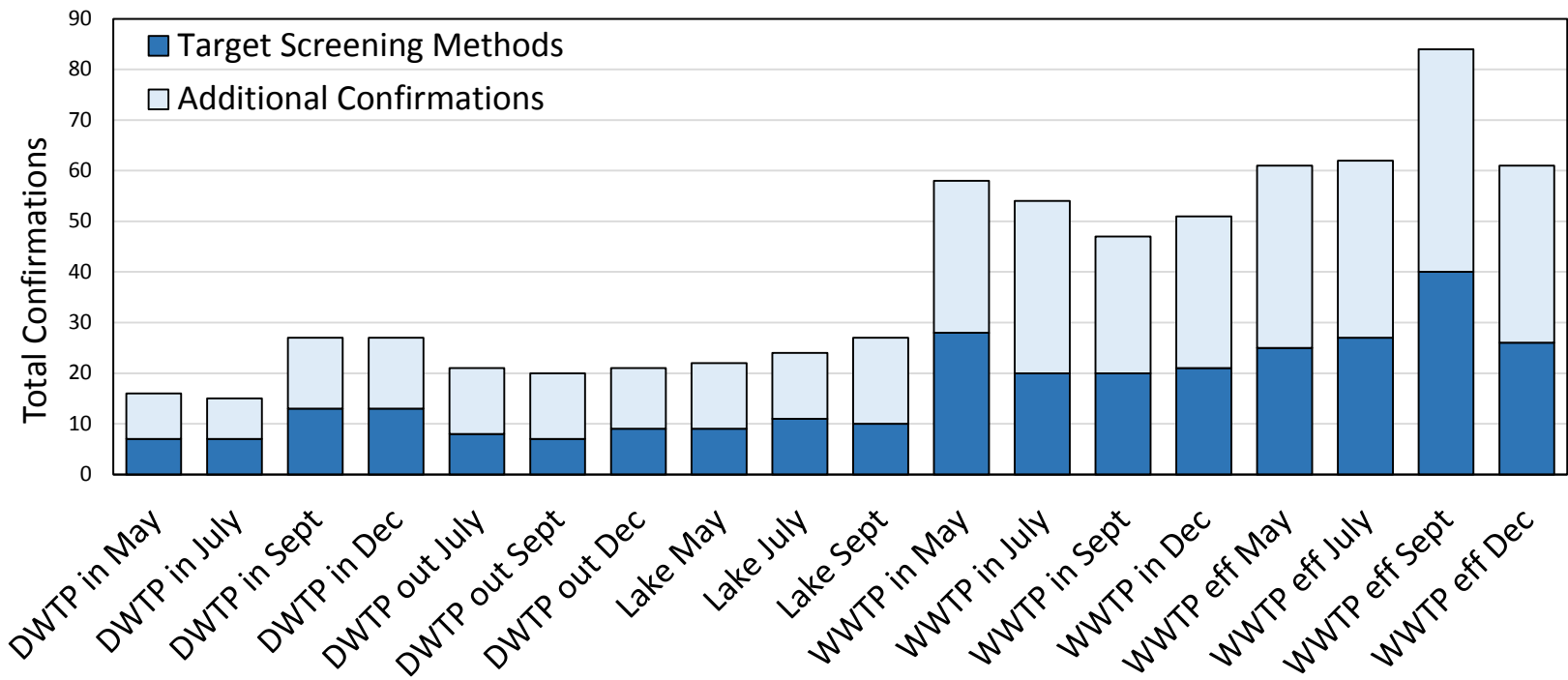


5-methyl-2H-benzotriazole

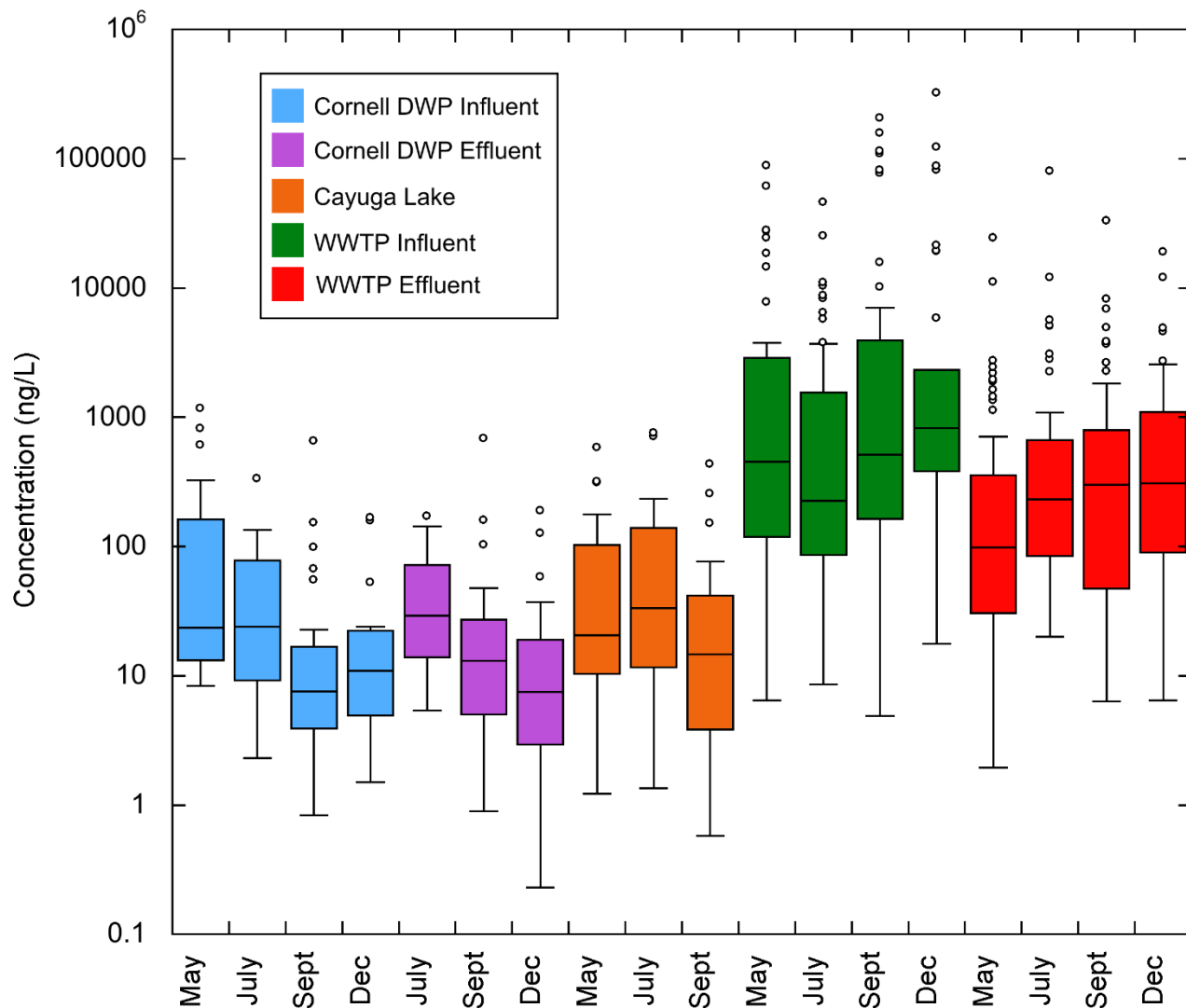


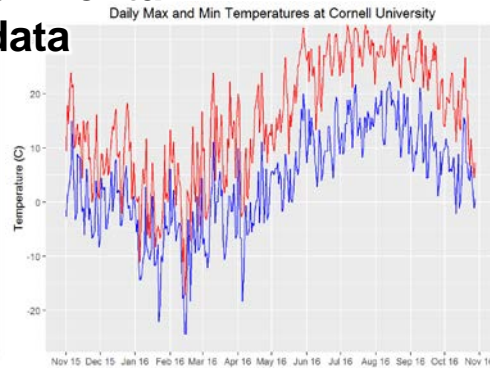
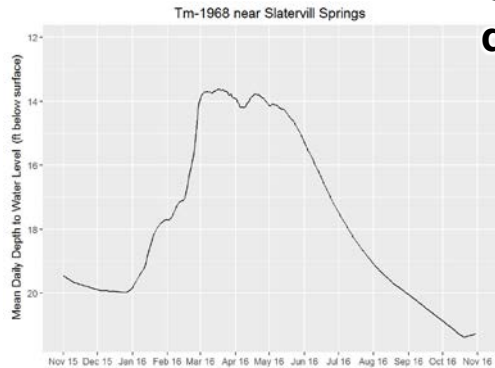
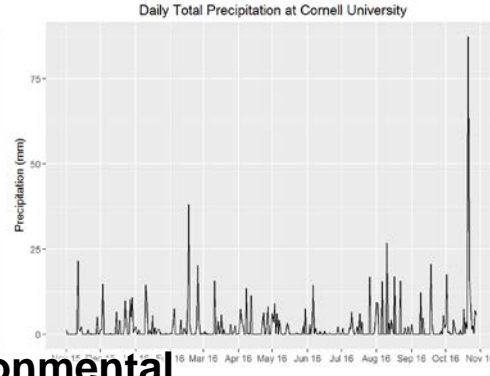
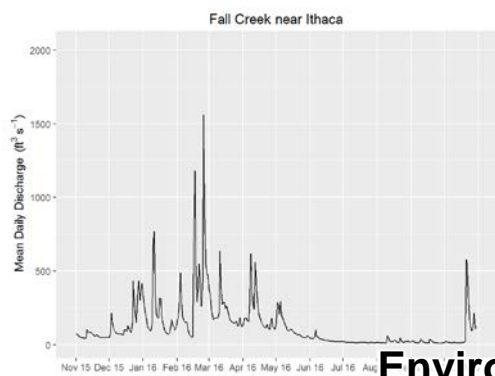
atenolol acid

Suspect screening – application



Results – concentrations of confirmed micropollutants

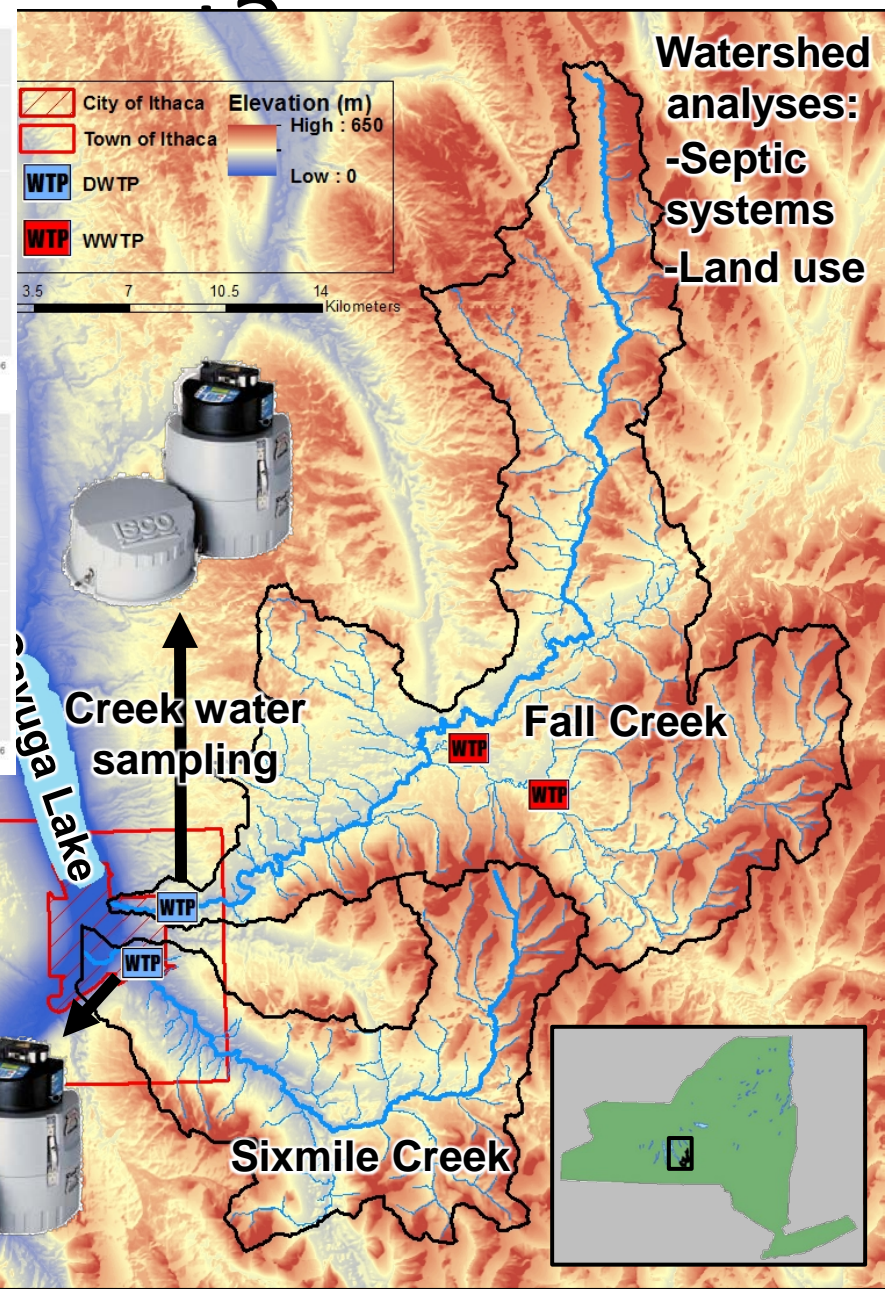
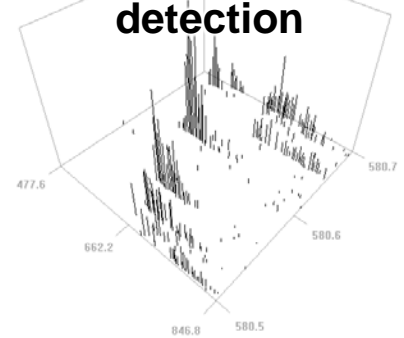




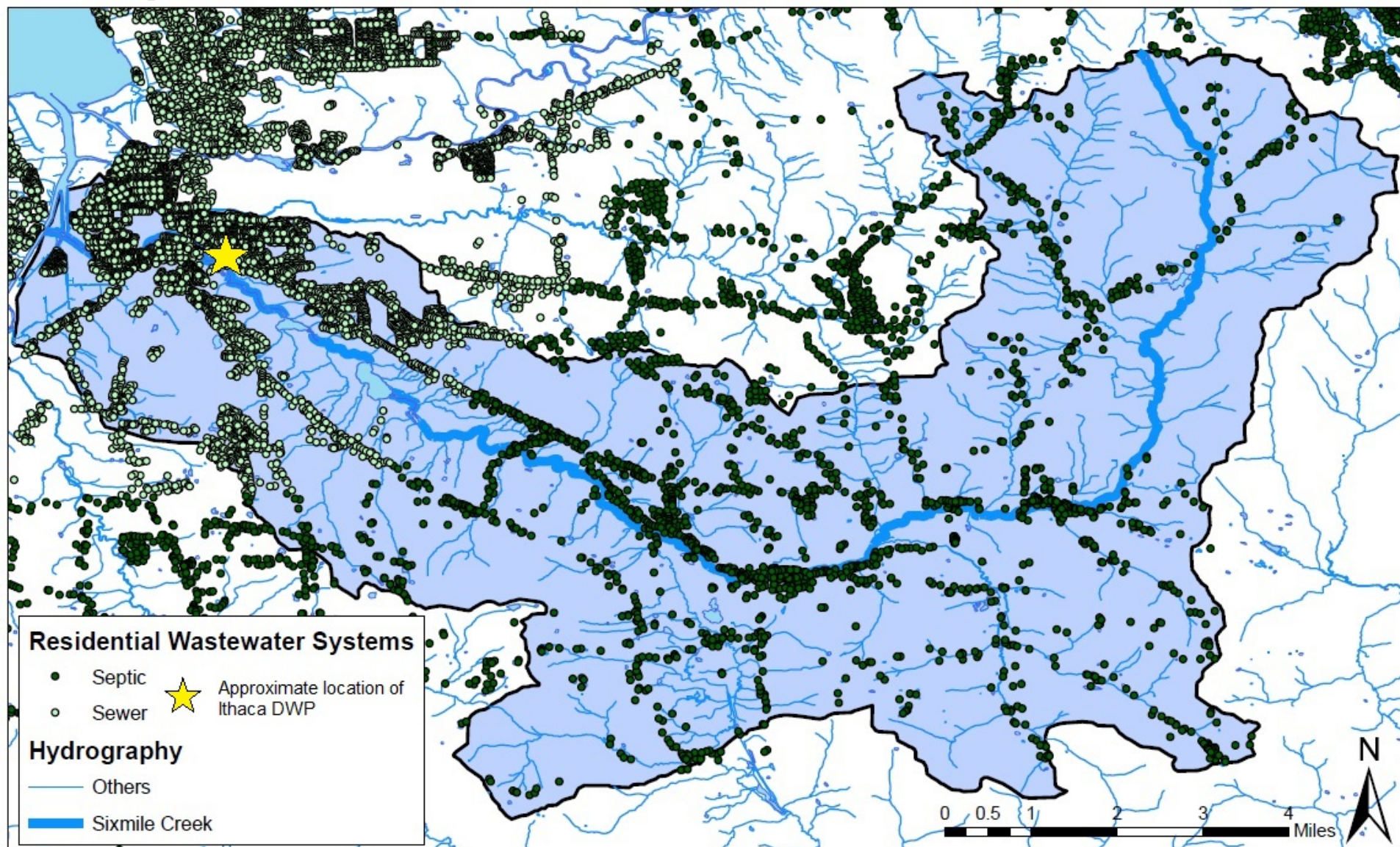
Environmental data

enviMass v3.1

Micropollutant trend detection



Example: Six Mile Creek watershed



Acknowledgements

<http://helbling.research.engineering.cornell.edu/>

Amy Pochodylo (Cornell)
Corey Carpenter (Cornell)
Jose Lozano (IAWWTF)
Chris Bordlemay (CWFP)
Patrick Phillips (USGS)
Tia-Marie Scott (USGS)
Susan Allen-Gil (Ithaca College)

