Prioritizing Pharmaceutical Contaminants in Great Lakes Tributaries Using Risk-Based Screening Techniques

Caffeine and nicotine were the chemicals most frequently prioritized according to screening-level benchmarks, but the toxicity of 48% of the detected chemicals remains undetermined.

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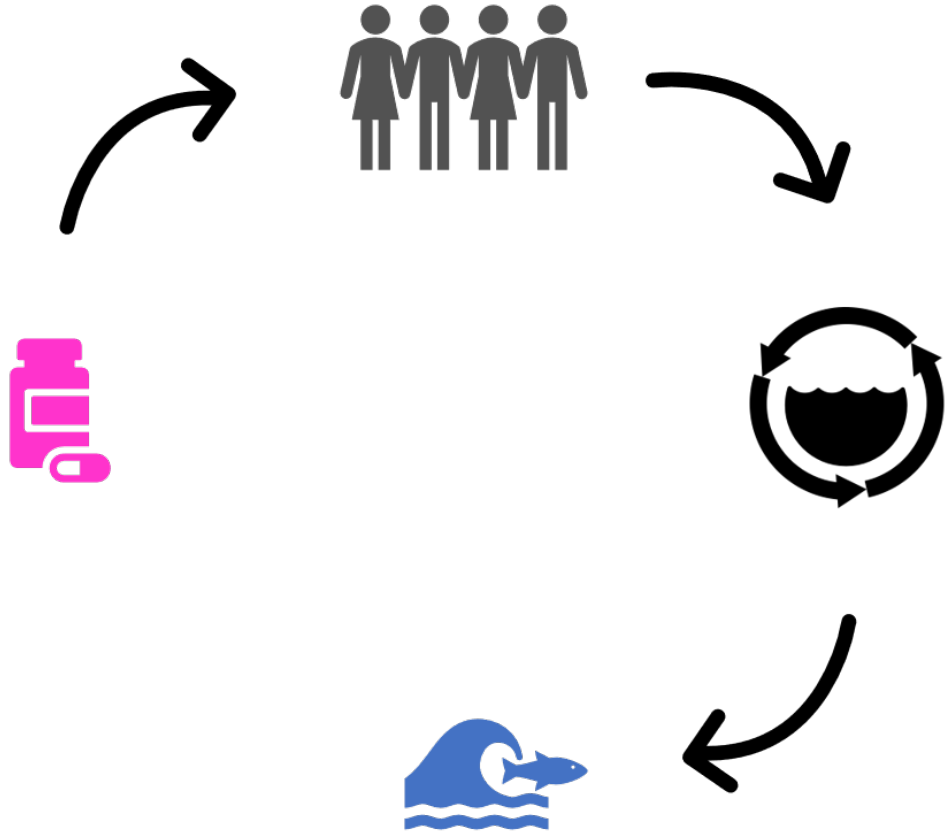
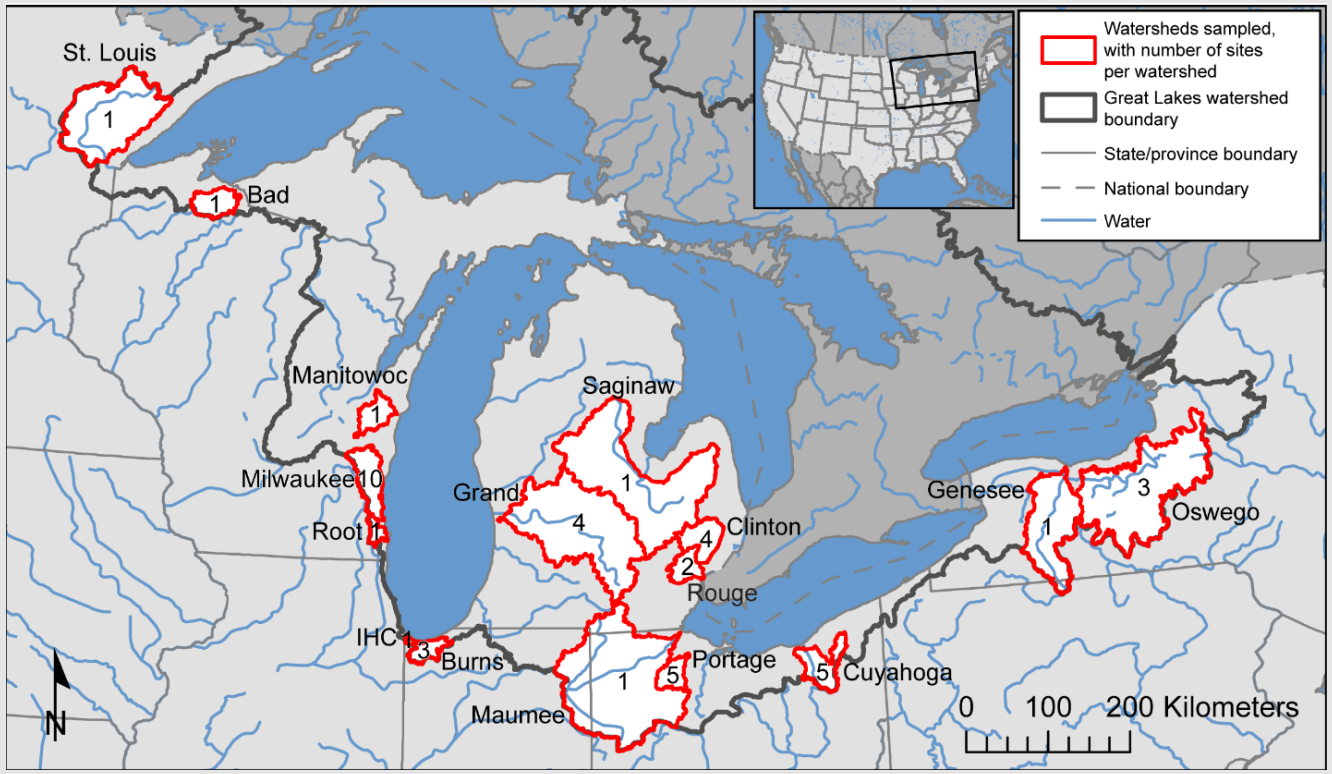
Where are pharmaceuticals?



Goals

1. Evaluate pharmaceutical prevalence
2. Evaluate the potential for adverse biological effects
3. Evaluate which chemicals are of greatest concern

Great Lakes pharmaceutical monitoring



Sampling design

- 113 water samples collected
- Up to 261 pharmaceutical analytes
  - 110 in Method 1
  - 151 in Method 2
- 44 tributary streams monitored to capture diverse
  - Seasons
  - Hydrologic conditions
  - Landcover
  - Wastewater treatment plant influence levels

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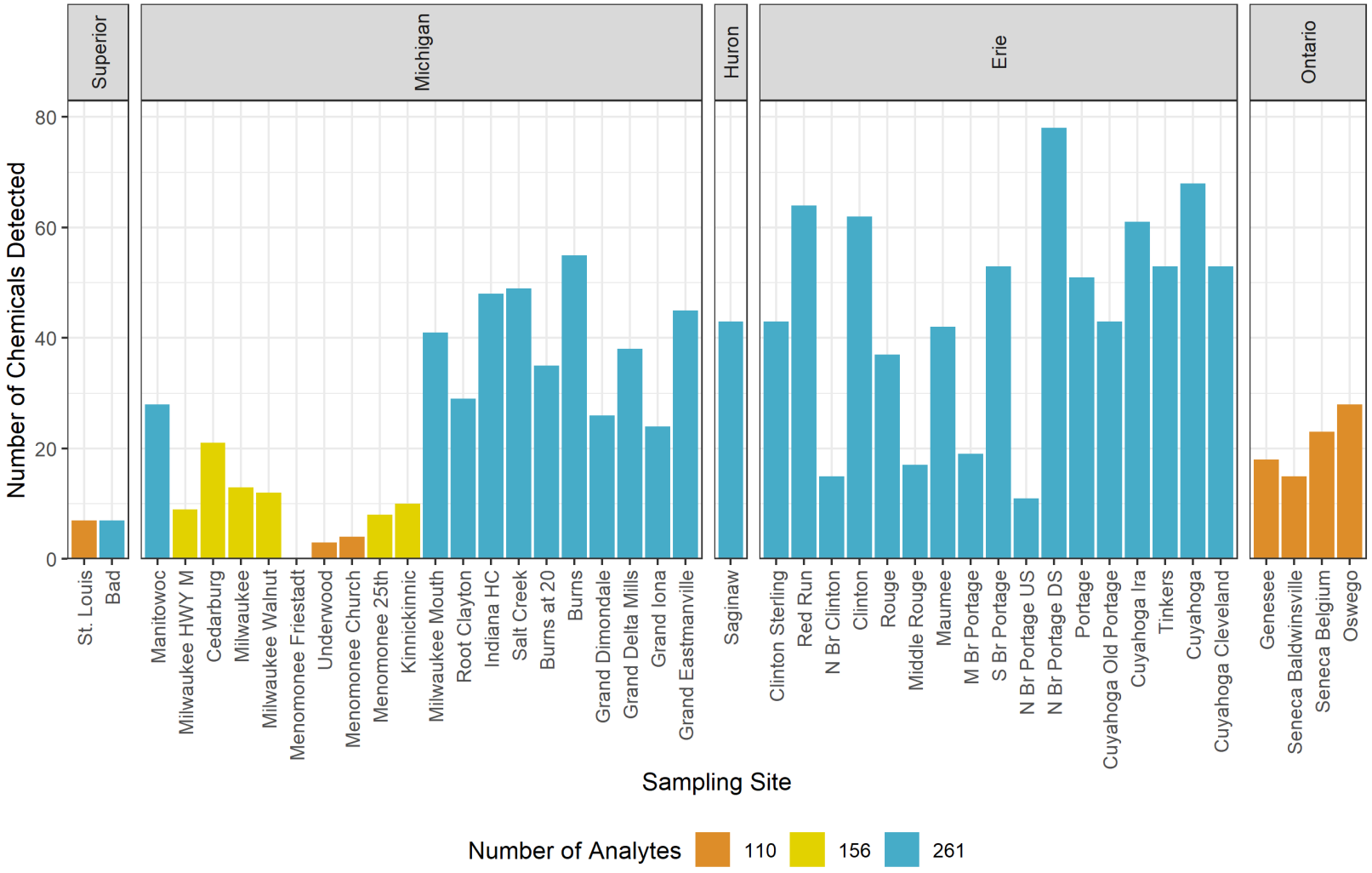
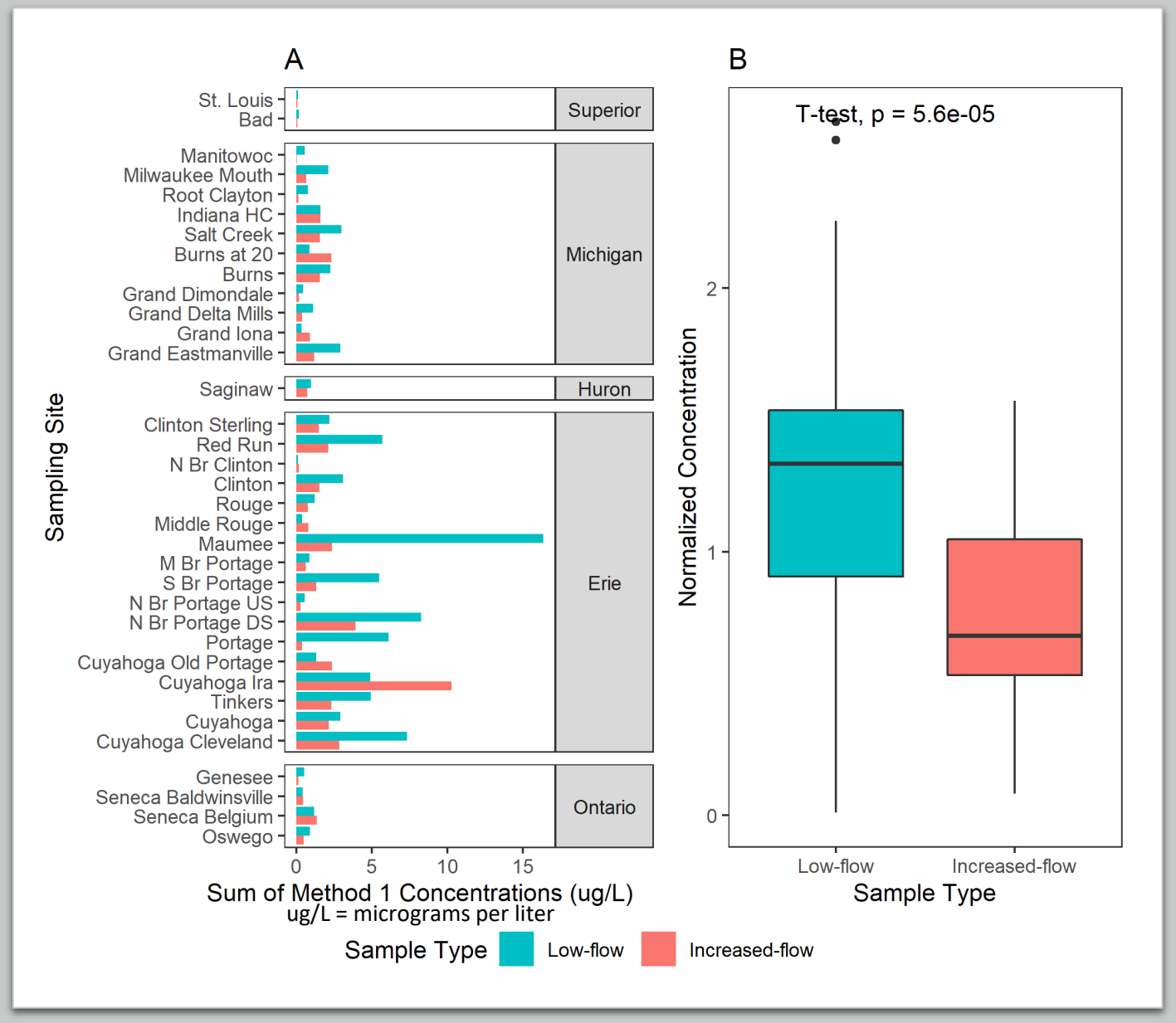
Pharmaceutical detections

- 113 chemicals detected
- Detections ranged from 0 to 78 per site
- Not all sites were monitored for all analytes
- High degrees of variation even among sites along the same waterway



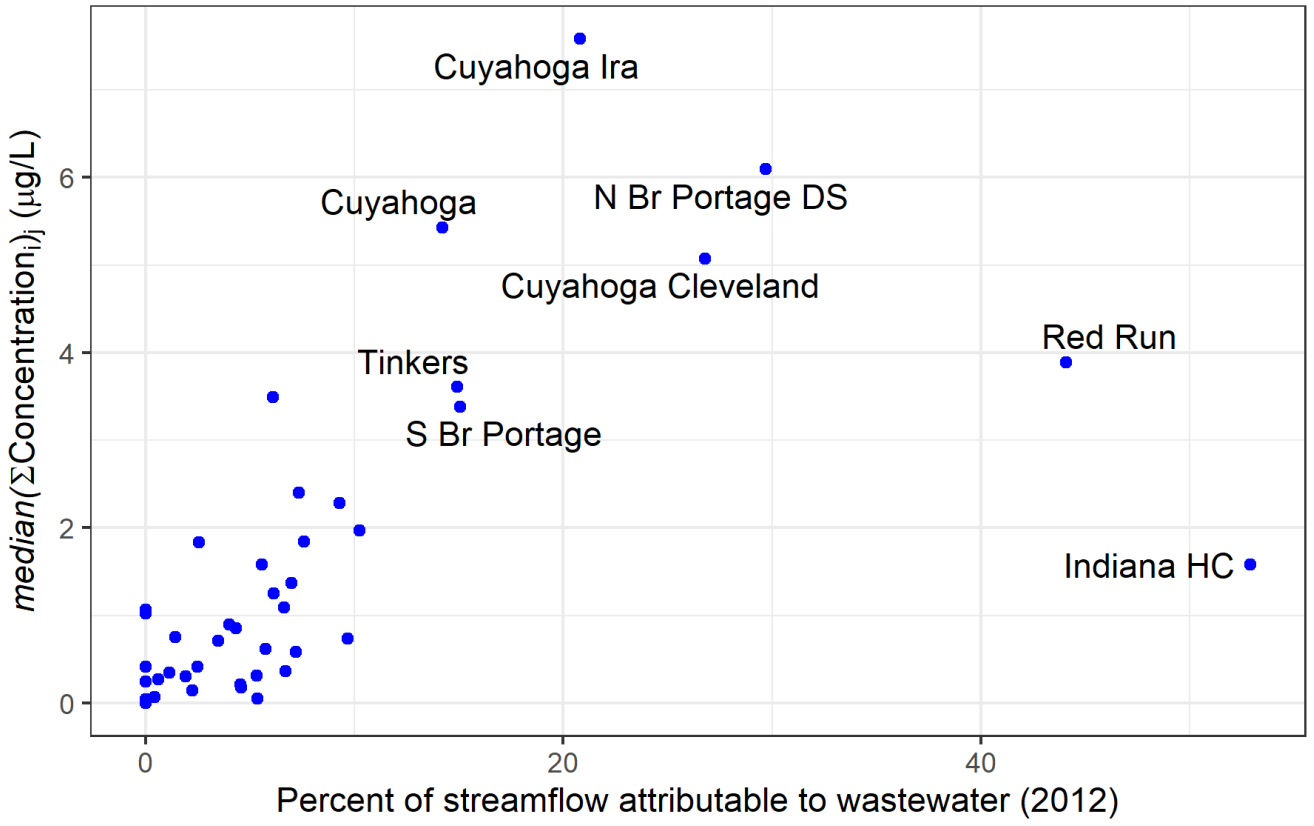
Hydrologic influence

- Low-flow samples had significantly higher pharmaceutical concentrations
- Increased flow serves to “dilute” pharmaceutical concentrations in streams



Wastewater influence

- Increased levels of wastewater treatment plant effluent correlates significantly with increased pharmaceutical concentrations
- Outliers: Red Run and Indiana HC (Harbor Canal) are situated in highly industrial watersheds; do industrial wastewaters “dilute” pharmaceutical concentrations?
- Wastewater treatment plants are not the only source of pharmaceutical compounds



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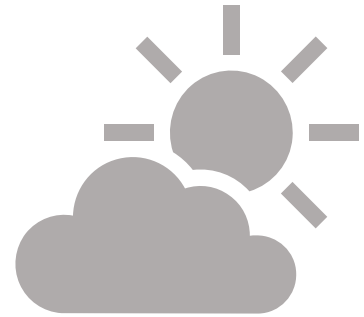
Which pharmaceutical compounds matter to aquatic life?

Challenges

- Countless pharmaceuticals to monitor; 261 in this study alone
- Lack of toxicity benchmarks
- Varying levels of chemical potency

(Partial) Solutions

- Toxicity Forecaster (ToxCast)
- ECOTOXicology Knowledgebase (ECOTOX)



Assessing biological relevance

ToxCast

- Consistent set of high-throughput screening assays
- Effects on cells, mitochondria, receptors, proteins, enzymes, DNA, RNA, etc.
- Activity Concentration at Cutoff → Exposure-Activity Ratio (EAR)

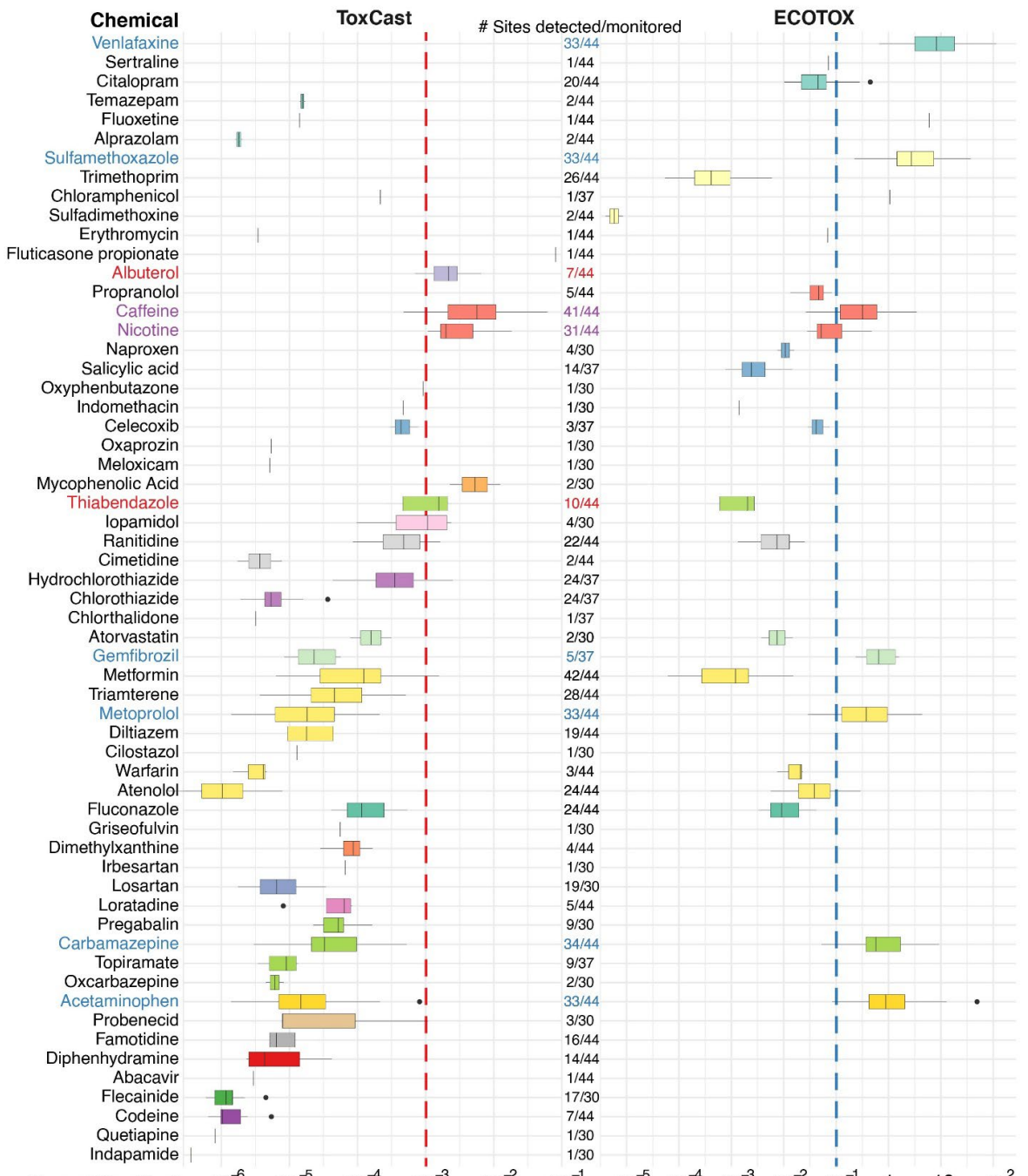
ECOTOX

- Vast knowledgebase of diverse toxicity studies and experiments
- Primarily whole-organism experiments
- Endpoint concentration → Toxicity Quotient (TQ)

$$\text{Hazard Quotient} = \frac{\text{Measured concentration in sample}}{\text{Water quality benchmark}}$$

Hazard Quotients

- Both sets of hazard quotients ranged many orders of magnitude
- Thresholds
  - Exposure-Activity Ratio = 10^{-3}
  - Toxicity Quotient = 0.1

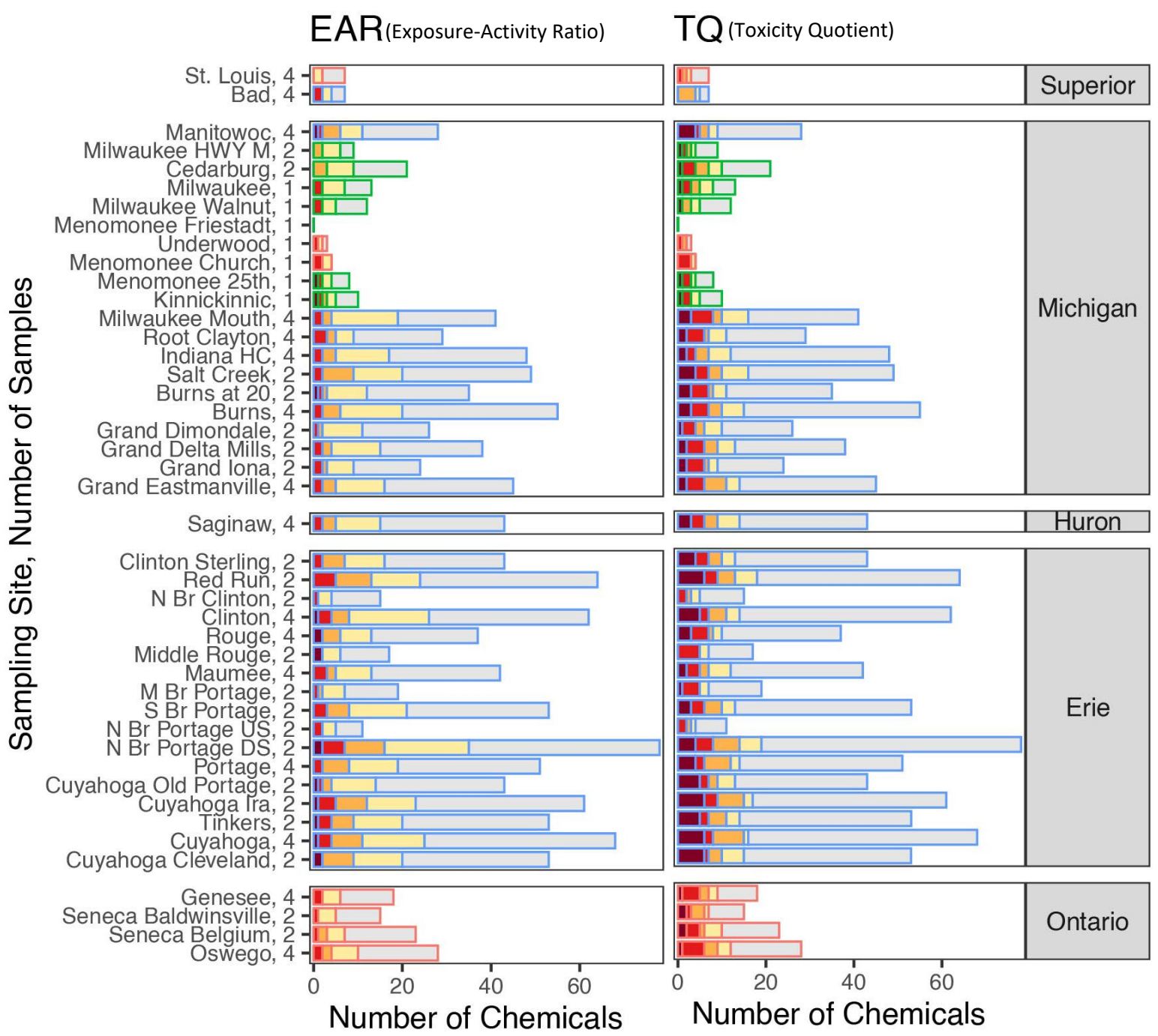


Class
Antidepressant
Antibiotic
Asthma Relief
Stimulant
NSAID
Immunosupressant
Anthelmintic
X–ray contrast agent
Antacid
Diuretic
Anticholesteremic
Cardiovascular Care
Antifungal
Degradate
Antihypertensive
Antiallergen
Anticonvulsant
Analgesic
Antigout
Chronic Condition
Antihistamine
Antiviral
Antiarrhythmic
Opioid
Antipsychotic
Antihyperglycemic

Preliminary Information-Subject to Revision. Not for Citation or Distribution.

Threshold exceedances

- Sites with at least one chemical exceeding a threshold:
  - EAR: 40 of 44
  - TQ: 42 of 44



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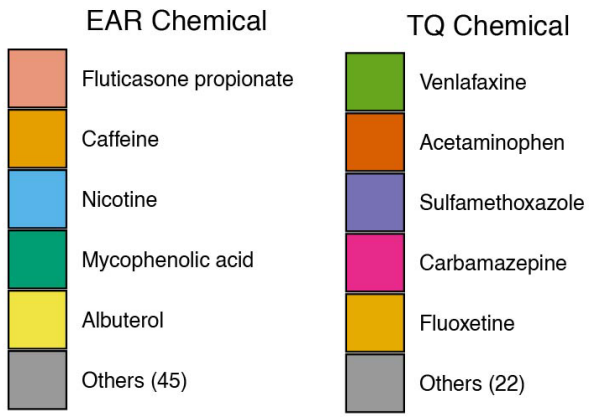
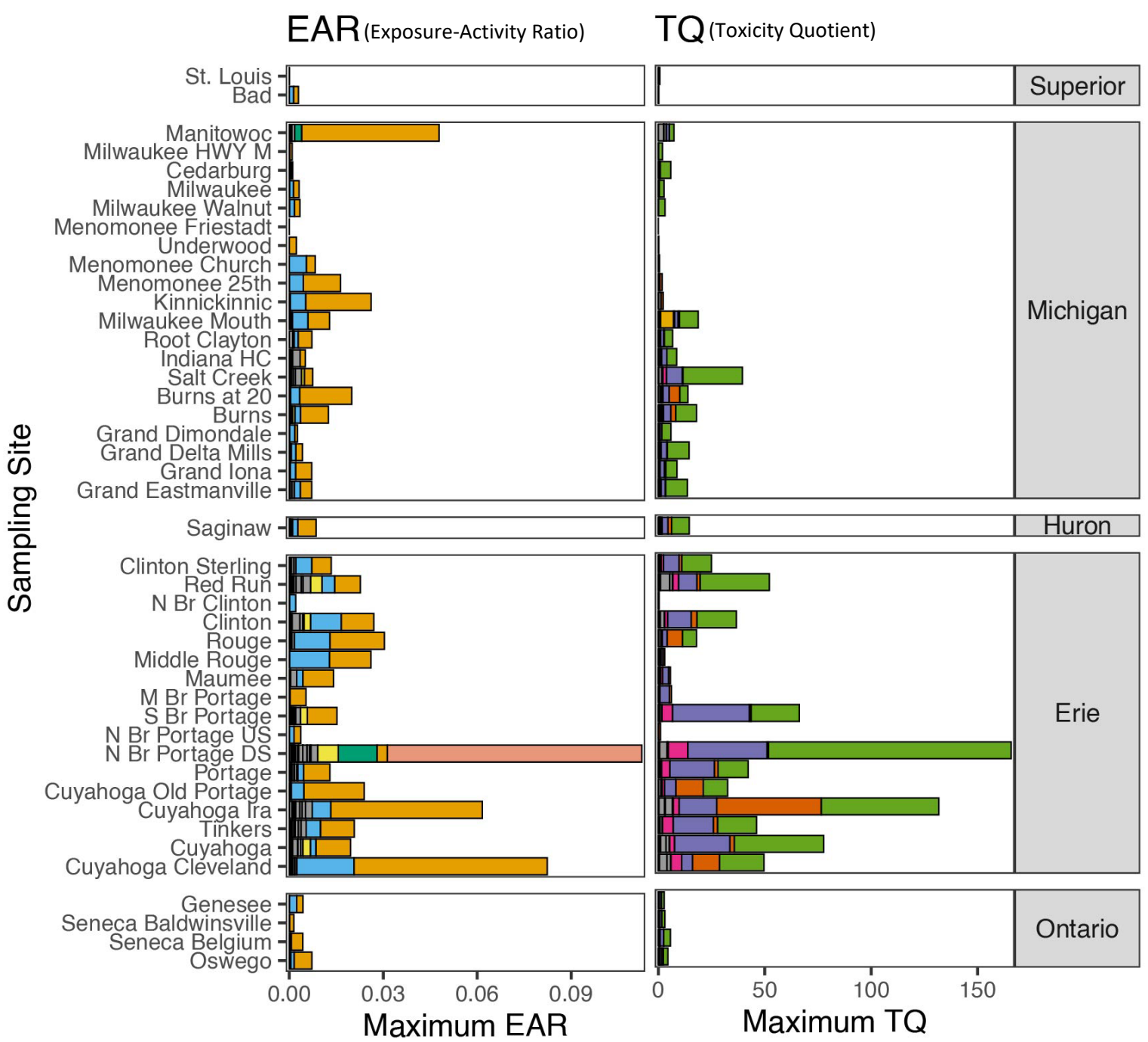
Chemical priorities

	Exceedances by Site	
Chemical	ToxCast EAR	ECOTOX TQ
Caffeine	**38**	**34**
Nicotine	**31**	**13**
Carbamazepine	0	33
Sulfamethoxazole	--	33
Venlafaxine	--	33
Acetaminophen	0	31
Metoprolol	0	29
Thiabendazole	6	0
Albuterol	5	--
Gemfibrozil	0	5





Conclusions

- Low-flow concentrations > increased-flow concentrations
- Water treatment plant effluent content correlates positively with concentrations
- Caffeine and nicotine were most frequently prioritized
- Venlafaxine, acetaminophen, and sulfamethoxazole dominated Toxicity Quotients
- More research needs to be conducted to put together the full puzzle

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