Understanding Spatial and Temporal Patterns of Contaminants in the Maumee River to Assess Biological Hazards

Dan Rearick
rearick.daniel@epa.gov
GDIT

Rearick, DC[Δ], Ankley GT[‡*]. Berninger, JP[‡], Blackwell B[‡], Cavallin JE[‡], Fay, KA[‡], Jensen KM[‡], Kahl MD[‡], Poole S[‡], Randolph E[‡], Schroeder A[†‡], Swintek, J[∞], Villeneuve DL[‡]

Great Lakes Restoration Initiative:
Contaminants of Emerging Concern (2010-Present)

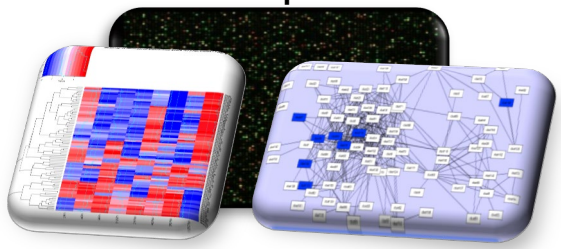
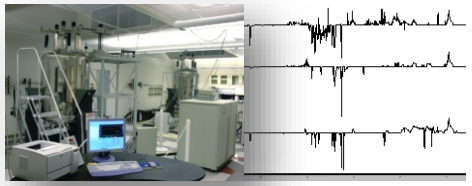
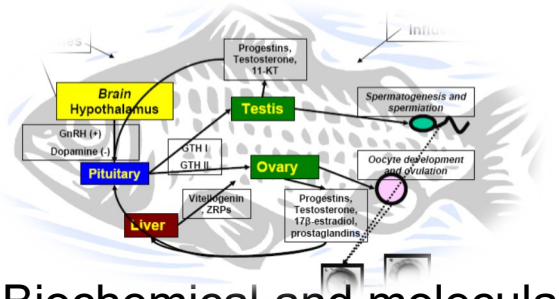
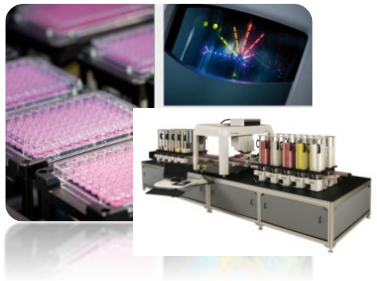
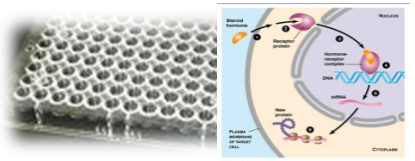
Objectives:

- To protect and restore the largest fresh surface water system in the world
- Identify emerging contaminants and assess impacts on Great Lakes fish and wildlife

Contaminants of Emerging Concern:

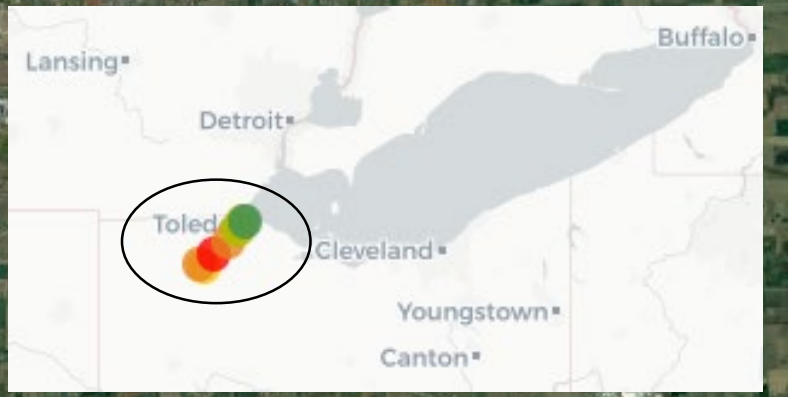
- Lacking exposure and/or effects data needed to support risk management
  - Current use pesticides, pharmaceuticals and personal care products, industrial chemicals, endocrine disruptors, other contaminants

Bioeffects Monitoring Approaches

	General Approach	Unsupervised	Supervised
In vivo assessment	Fish exposed in situ 	DNA-microarray Transcriptomics  Metabolomics 	• Endpoints associated with established adverse outcome pathways:  • E.g., Biochemical and molecular markers of endocrine disruption and adverse reproductive outcomes.
In vitro assessment	Surface water samples/extracts 	High throughput in vitro screening 	 In vitro bioassays • MDA-kb2: (anti)androgenic activity • T47D: (anti)estrogenic activity • H4IIE: dioxin-like contaminants • H295R: steroidogenesis inhibitors

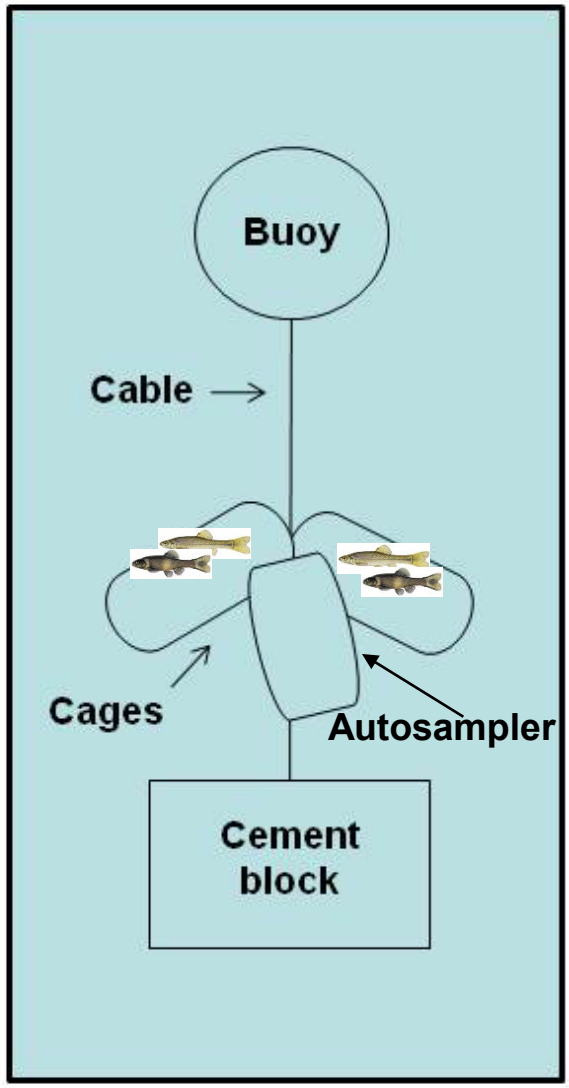
Maumee River AOC

- GLRI CEC project
- Characterize chemistry in a complex landscape
- Identify spatial patterns of chemical mixtures using **Cluster Analysis**
  - Seasonal trends in 2016
- Discuss implications to potential effects: **EAR** calculations using ToxEval: http://usgs-r.github.io/toxEval/articles/Introduction.html



Methods

- Autosampler co-located to collect 96h composite sample
  - Chemistry (WWI, pesticides, pharmaceuticals)
  - Bioassays (Attagene, estrogenic activity, cell-based metabolomics, steroidogenesis, ZF embryo transcriptomics)
- Caged fish deployed at sites; 96h exposure period
  - Mucus (metabolomics)
  - Plasma (steroids, vtg)
  - Liver (gene expression, ‘omics)
  - Gonad (gene expression, ‘omics)

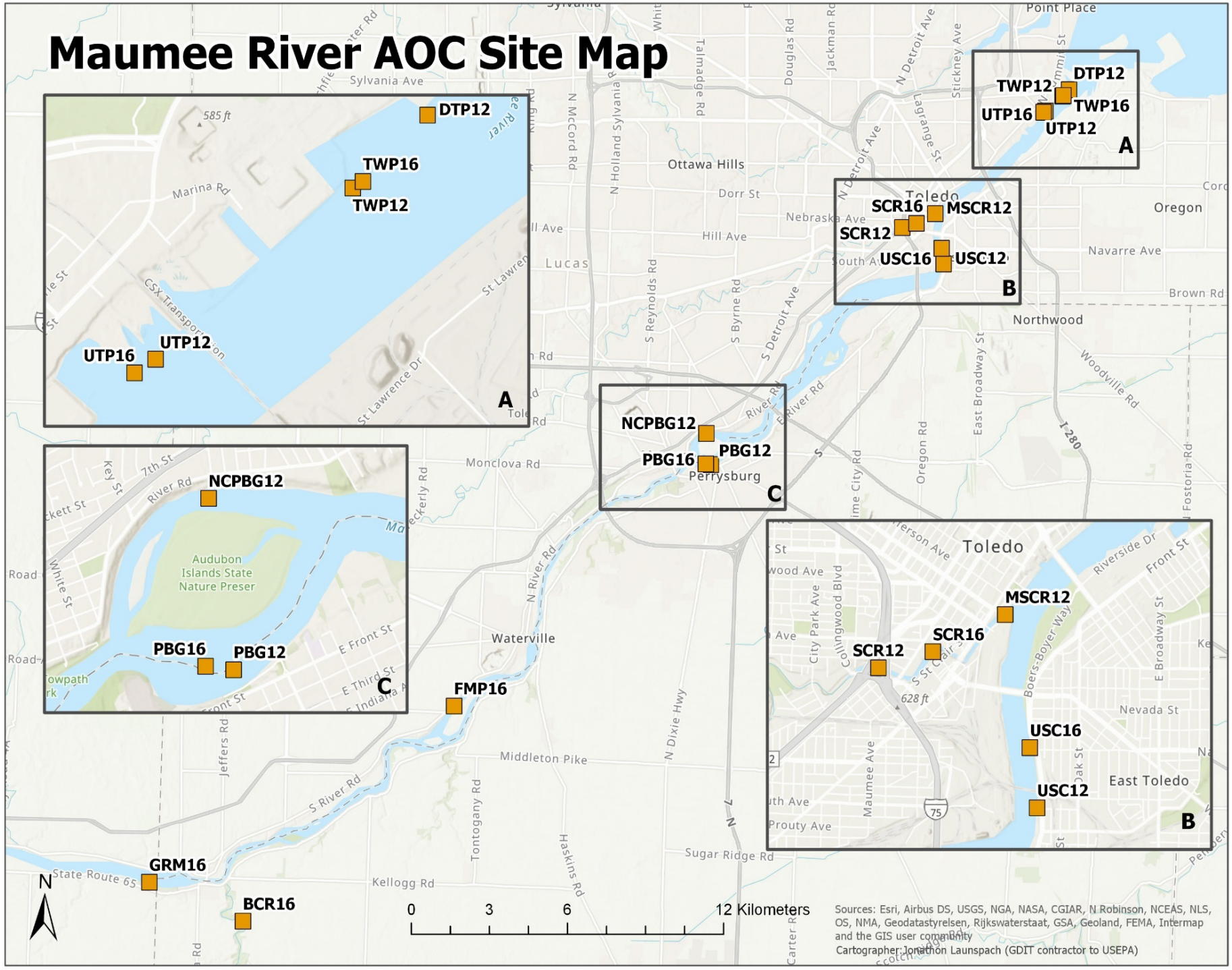


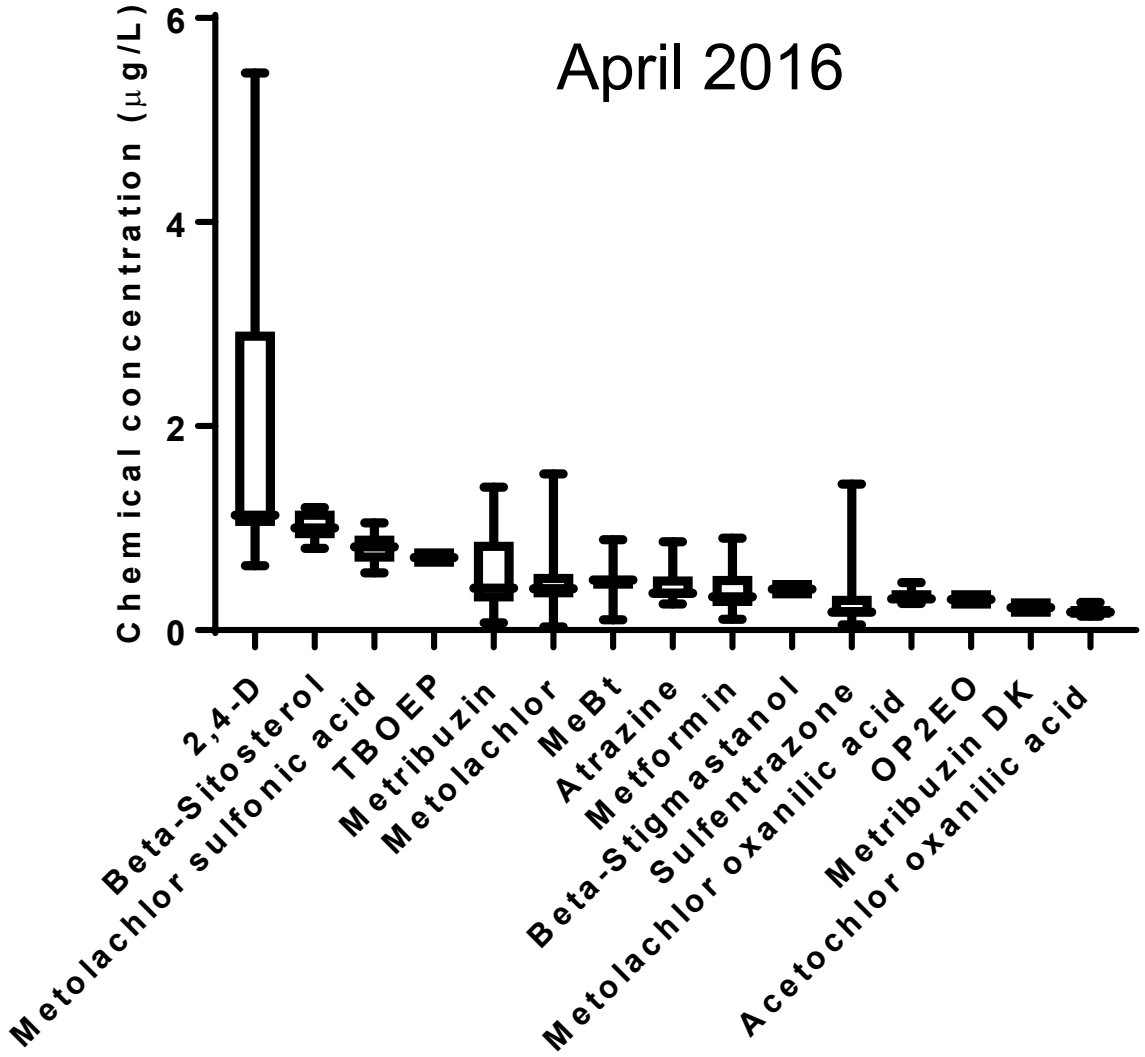
USGS Water Chemistry Schedules

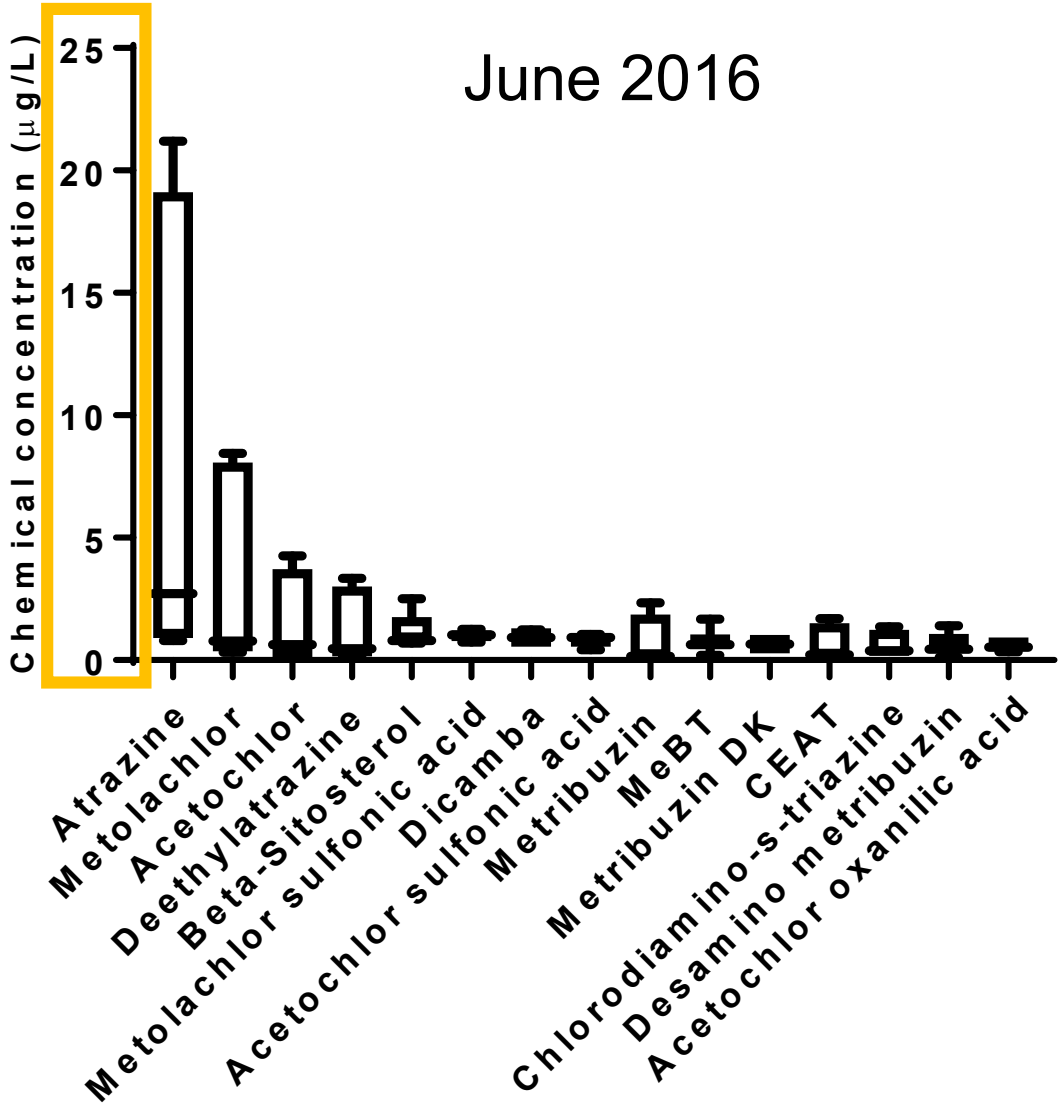
- Prior sampling (2012) revealed agricultural influence in the AOC
- Pre/post runoff pesticide application

April and June 2016

- Pesticides
- Pharmaceuticals
- Wastewater indicators







110-111 target chemicals detected

- Pesticides: 58-63
- Pharmaceuticals: 25-28
- Wastewater indicators: 22-25

Maumee River AOC

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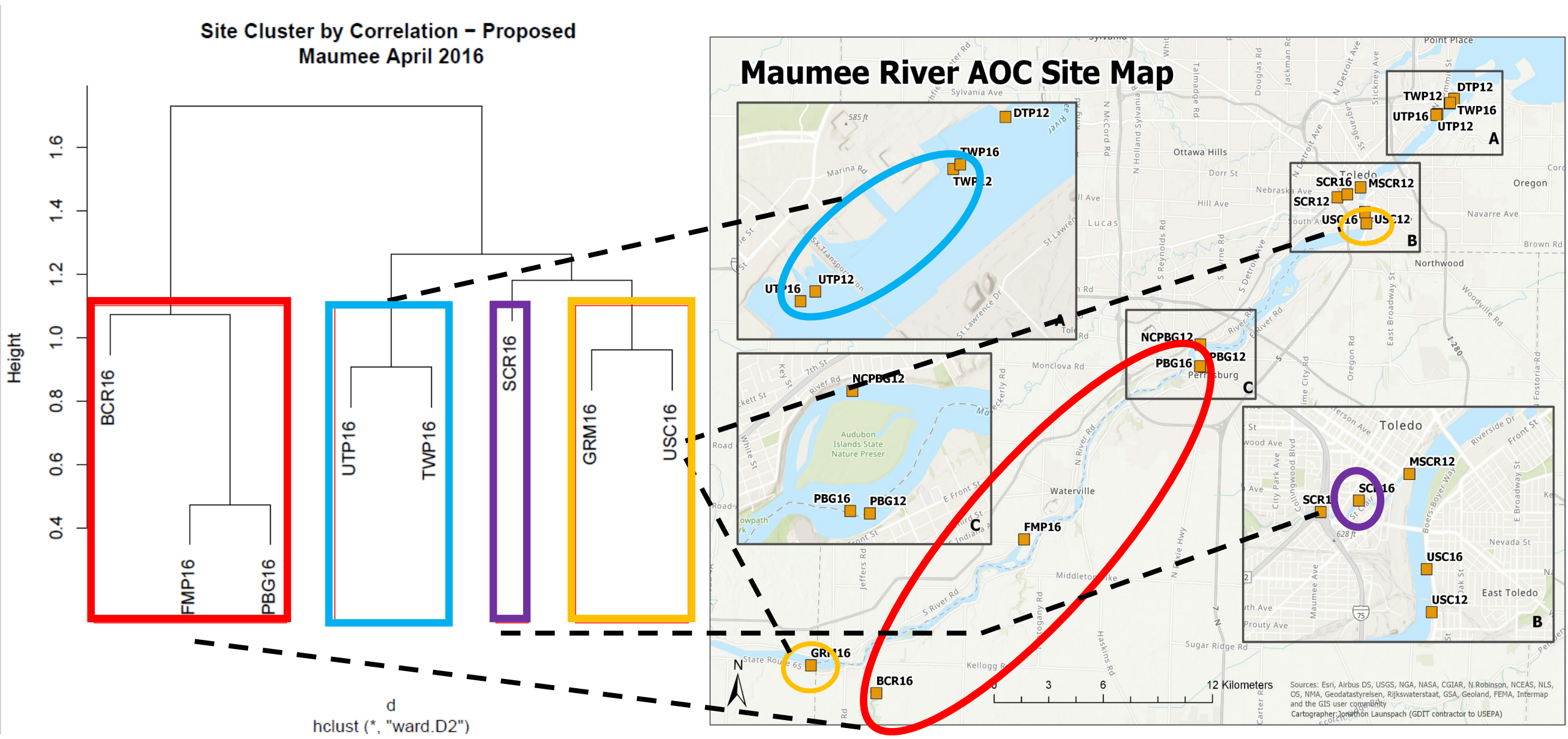
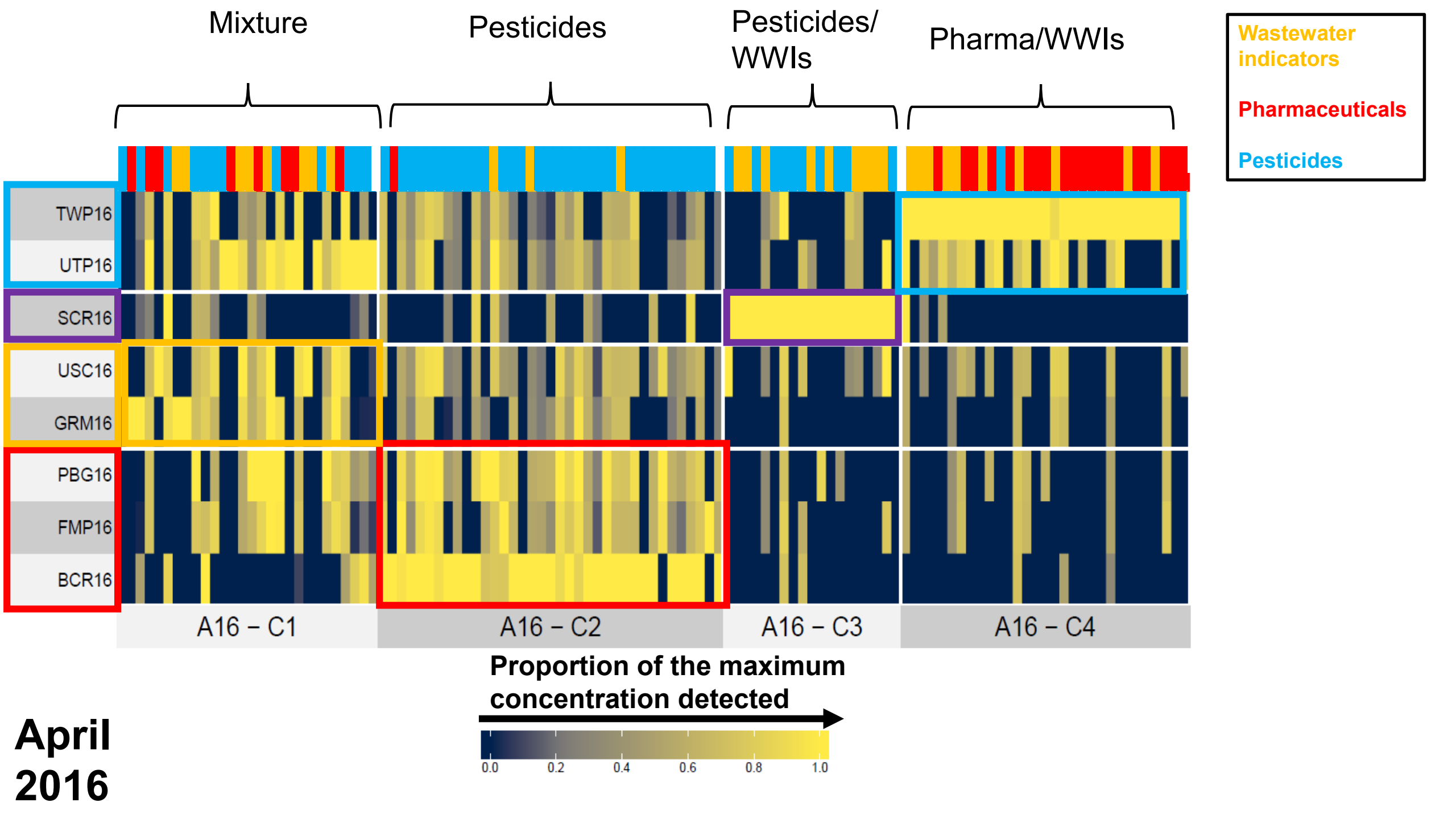
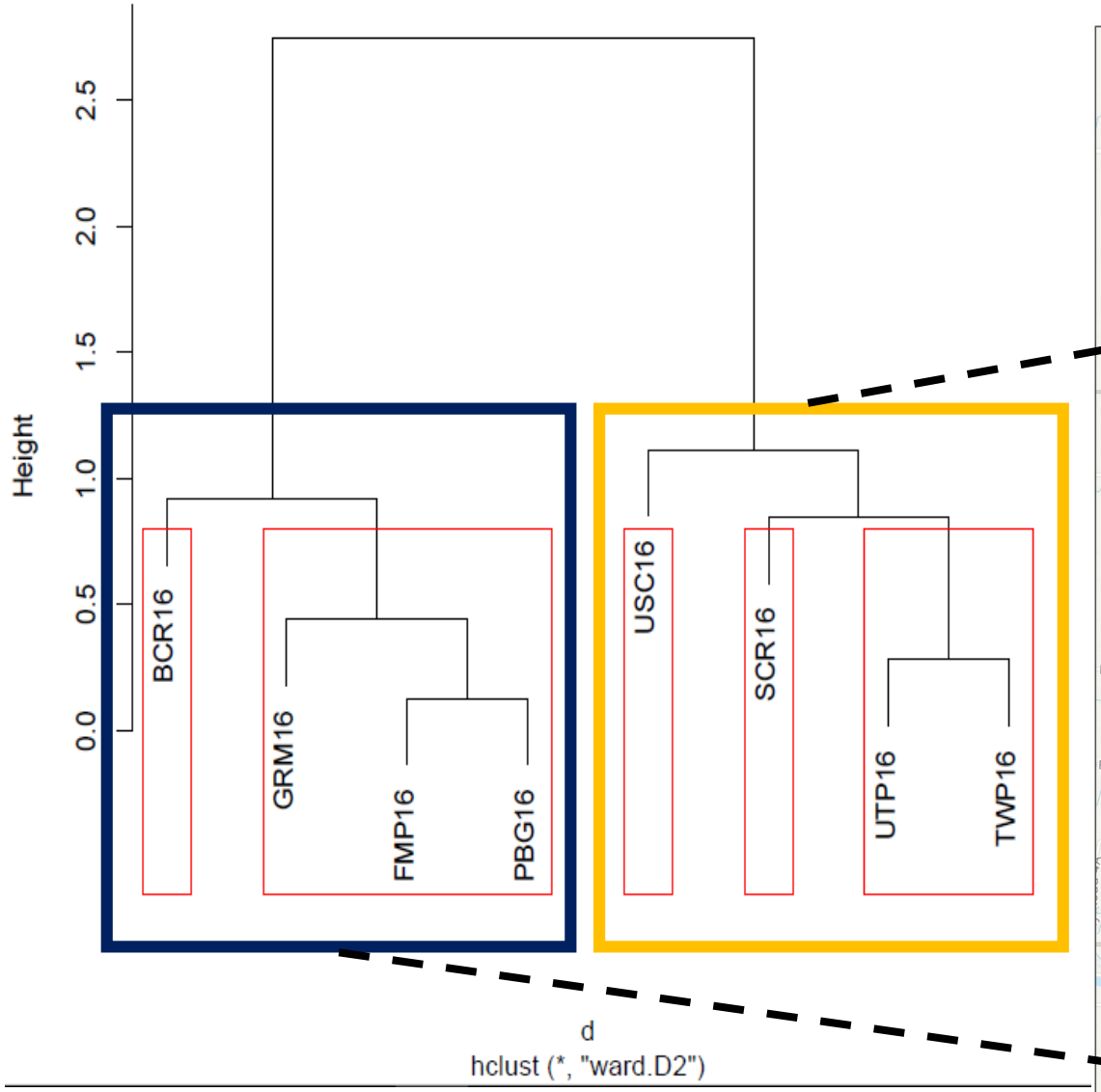
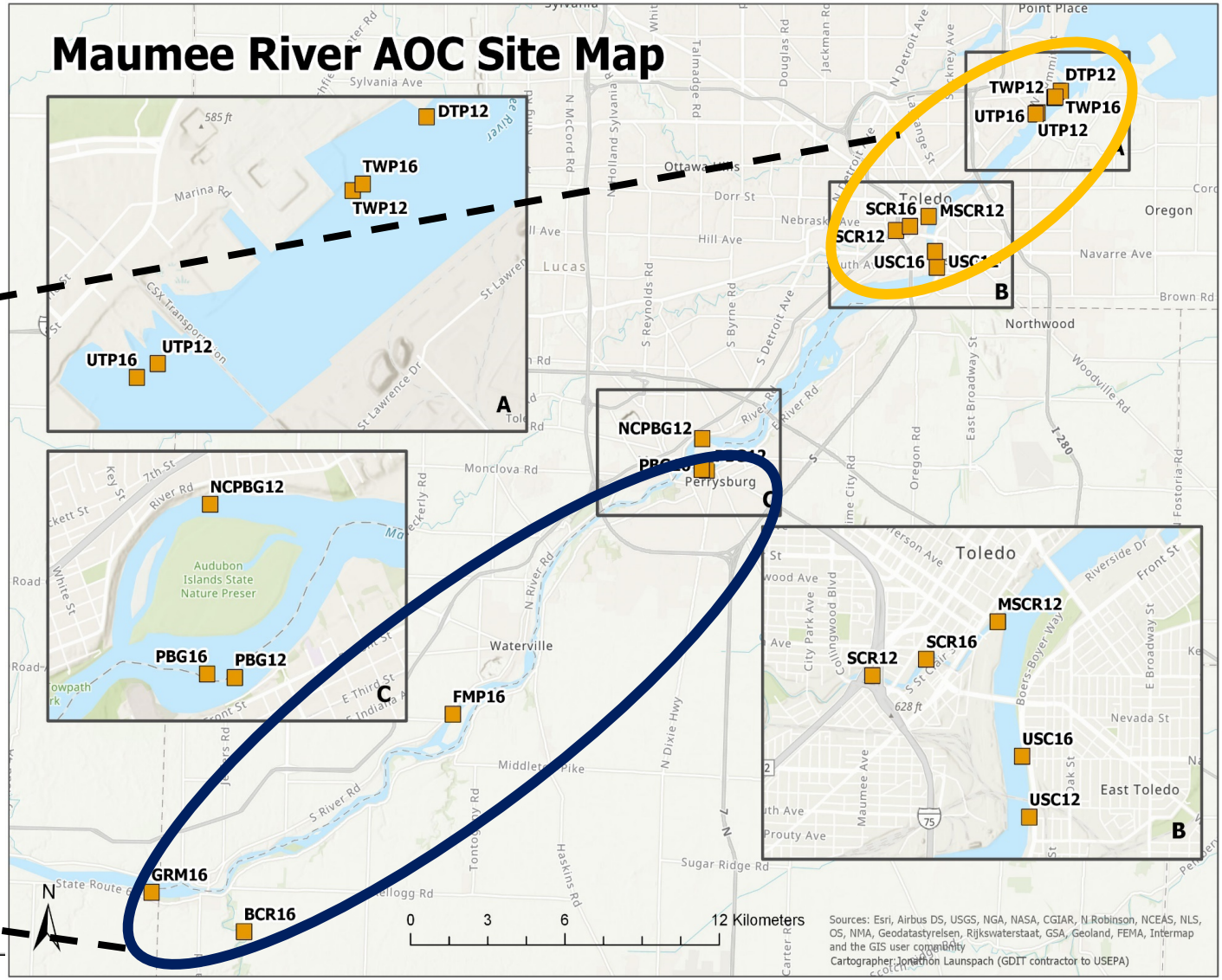
- Discuss implications to potential effects: **EAR** calculations using ToxEval: http://usgs-r.github.io/toxEval/articles/Introduction.html


Site Cluster by Correlation – Proposed
Maumee April 2016
Height
0.4
0.6
0.8
1.0
1.2
1.4
1.6
BCR16
FMP16
PBG16
UTP16
TWP16
SCR16
GRM16
USC16
d
hclust (*, "ward.D2")
Maumee River AOC Site Map
DTP12
TWP16
TWP12
UTP16
UTP12
A
SCR16
MSCR12
SCR12
USC16
USC12
B
NCPBG12
PBG16
PBG12
C
Audubon Islands State Nature Preser
Waterville
FMP16
Toledo
East Toledo
Ottawa Hills
Northwood
Oregon
Perrysburg
Monclova Rd
Sylvania Ave
Dorr St
Hill Ave
Nebraska Ave
Navarre Ave
Brown Rd
Woodville Rd
Nevada St
Sugar Ridge Rd
Kellogg Rd
S River Rd
N River Rd
E Front St
Jeffers Rd
Middleton Pike
N
0
3
6
12 Kilometers
Sources: Esri, Airbus DS, USGS, NGA, NASA, CGIAR, N Robinson, NCEAS, NLS, OS, NMA, Geodatastyrelsen, Rijkswaterstaat, GSA, Geoland, FEMA, Intermap and the GIS user community
Cartographer: Jonathon Launspach (GDIT contractor to USEPA)


Mixture
Pesticides
Pesticides/ WWIs
Pharma/WWIs
Wastewater indicators
Pharmaceuticals
Pesticides
TWP16
UTP16
SCR16
USC16
GRM16
PBG16
FMP16
BCR16
A16 – C1
A16 – C2
A16 – C3
A16 – C4
Proportion of the maximum concentration detected
0.0
0.2
0.4
0.6
0.8
1.0
April 2016


Height
2.5
2.0
1.5
1.0
0.5
0.0
BCR16
GRM16
FMP16
PBG16
USC16
SCR16
UTP16
TWP16
d
hclust (*, "ward.D2")


Maumee River AOC Site Map
DTP12
TWP16
TWP12
UTP16
UTP12
A
SCR16
MSCR12
SCR12
USC16
B
NCPBG12
Perrysburg
C
Audubon Islands State Nature Preser
PBG16
PBG12
FMP16
Waterville
Toledo
MSCR12
SCR16
SCR12
USC16
USC12
East Toledo
GRM16
BCR16
N
0
3
6
12 Kilometers
Sources: Esri, Airbus DS, USGS, NGA, NASA, CGIAR, N Robinson, NCEAS, NLS, OS, NMA, Geodatastyrelsen, Rijkswaterstaat, GSA, Geoland, FEMA, Intermap and the GIS user community
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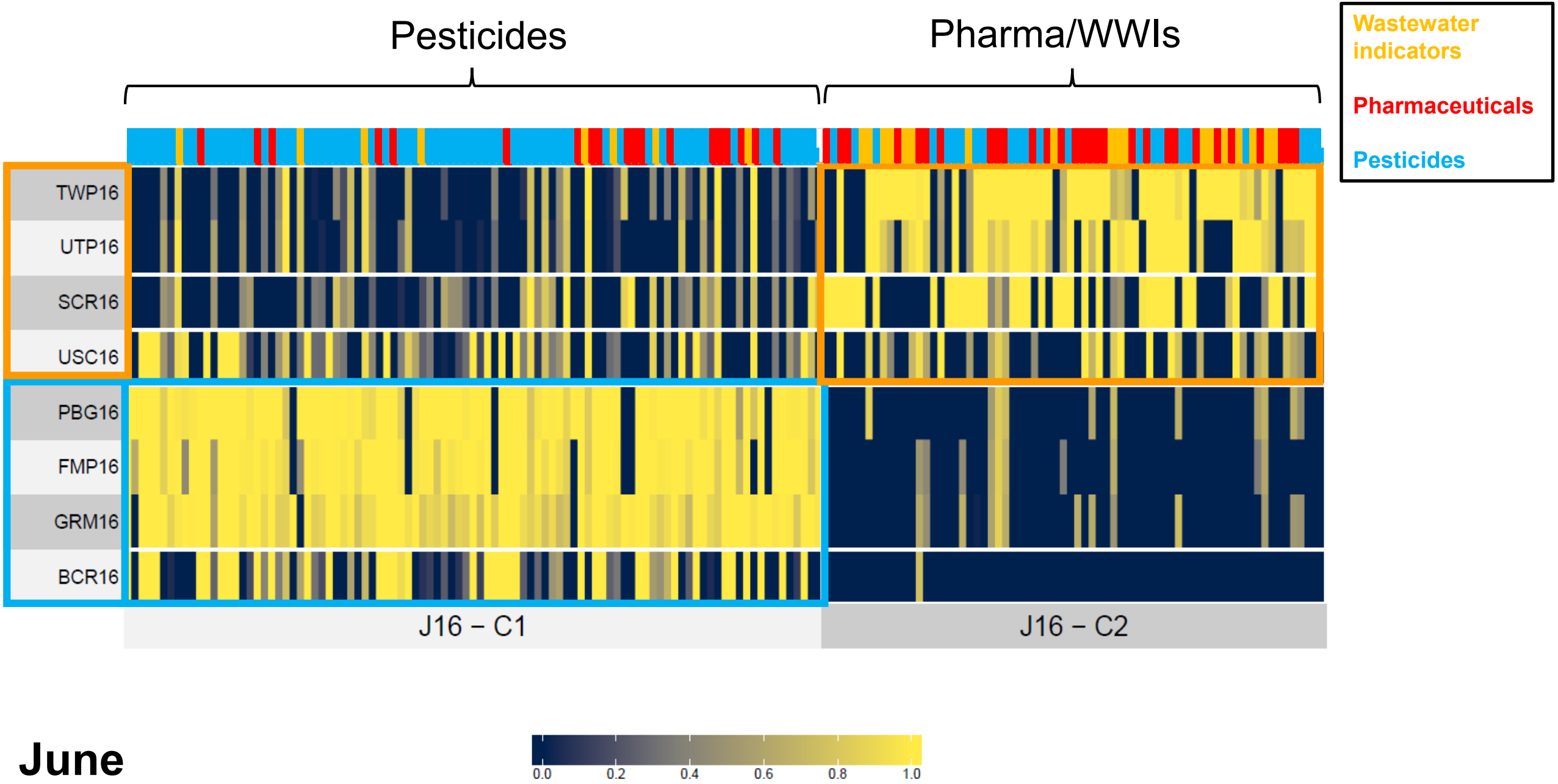

Pesticides
Pharma/WWIs
Wastewater indicators
Pharmaceuticals
Pesticides
TWP16
UTP16
SCR16
USC16
PBG16
FMP16
GRM16
BCR16
J16 – C1
J16 – C2
0.0
0.2
0.4
0.6
0.8
1.0

June 2016

High-throughput Screening (HTS) based predictions using Exposure-Activity Ratios

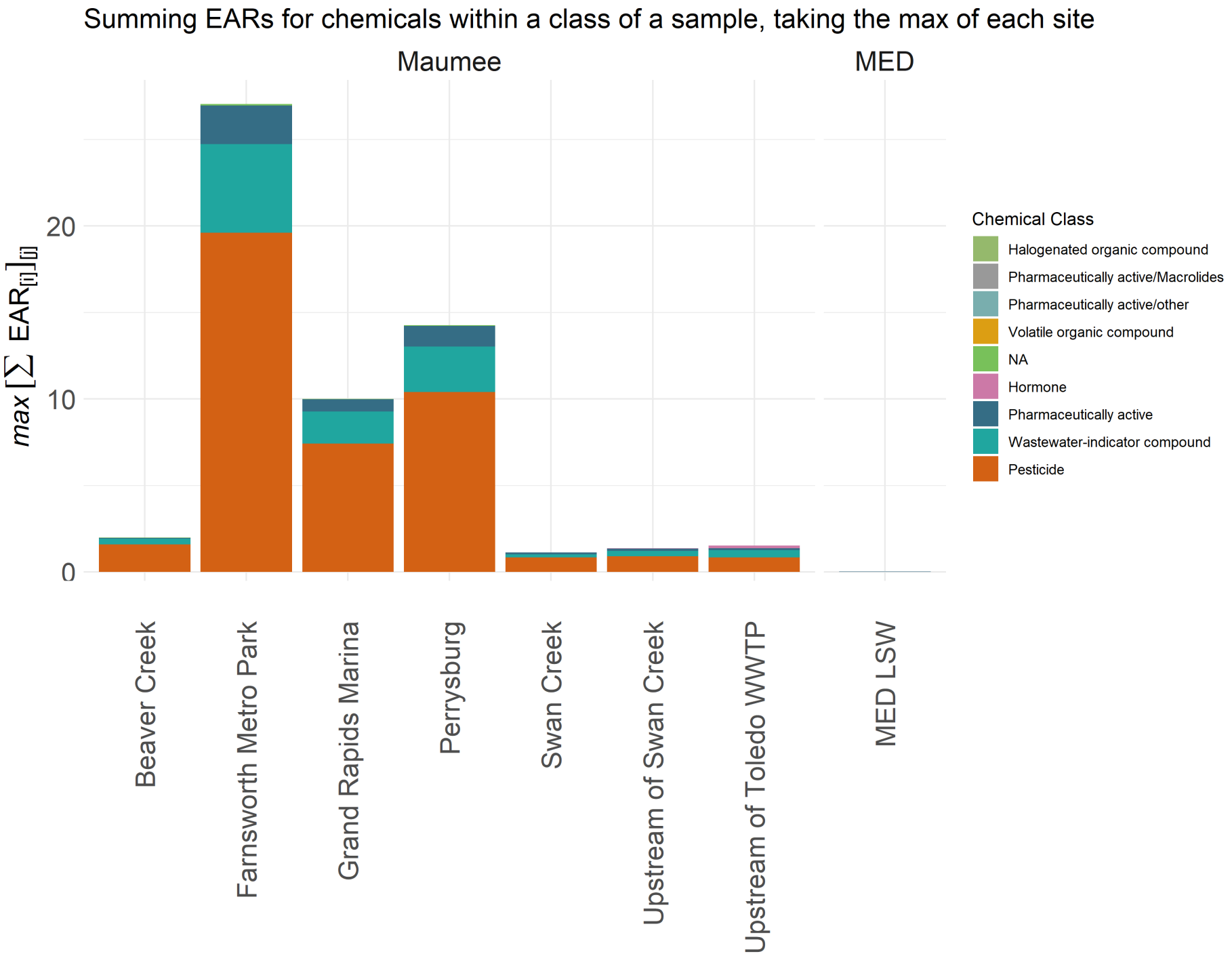
- R-based tool to compare chemical occurrence data with ToxCast database
  - ToxCast database contains biological activities for 1000s of chemicals
  - HTS includes cell-based and biochemical *in vitro* assays to investigate chemical-biological interactions
  - Exposure activity ratios provide hazard predictions using chemical potency to determine adverse effects on biological activity
  - Allows for prioritization of sites, chemicals, and biological pathways

- We present maximum concentrations detected in 2016 for both seasons tested

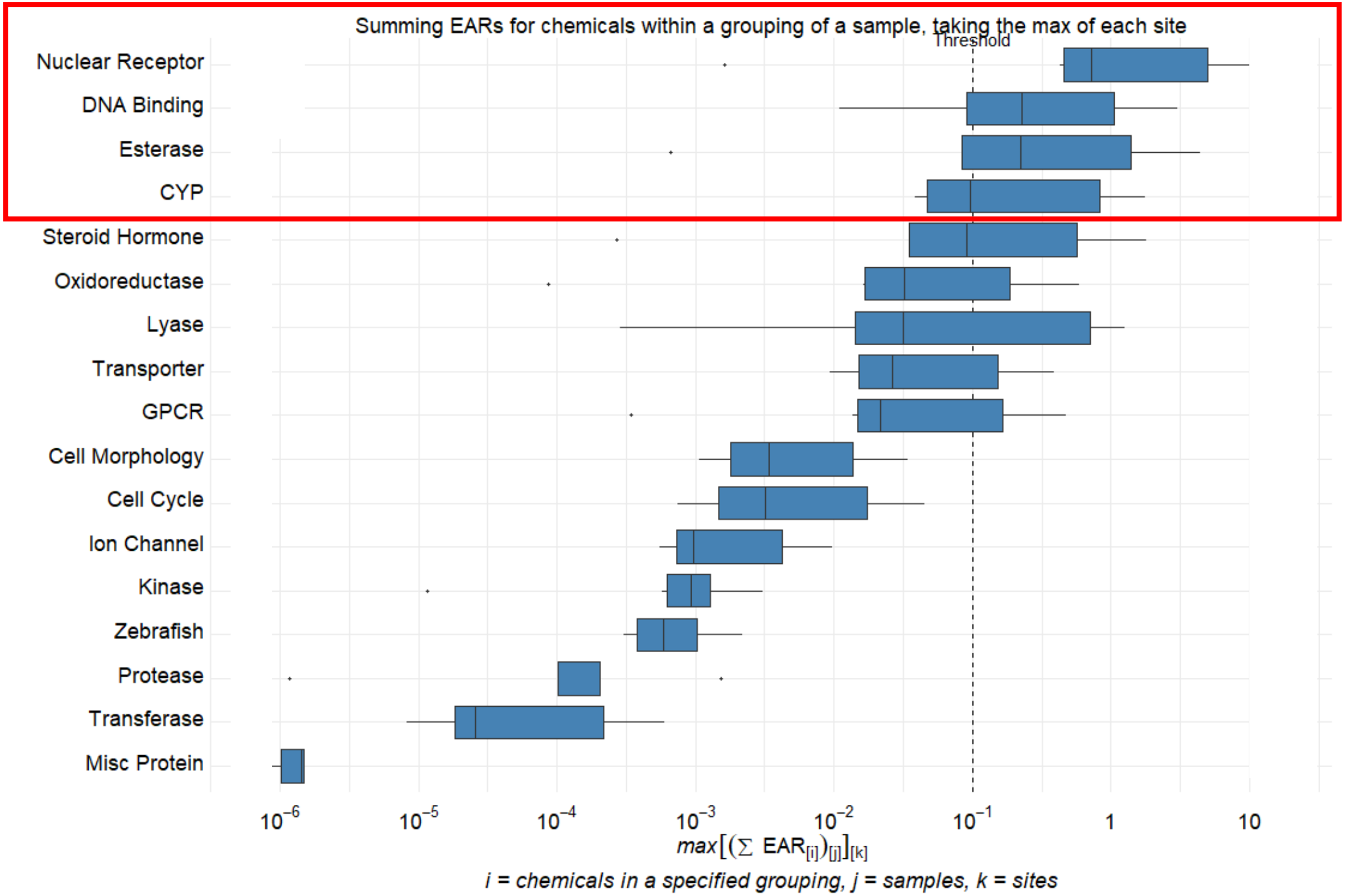
$$\text{EAR mixture} = \sum_{i=1}^{n} \frac{\text{Exposure}_i(\text{dose uM})}{\text{Activity}_i(\text{ACC uM})}$$

Pesticides are major contributor

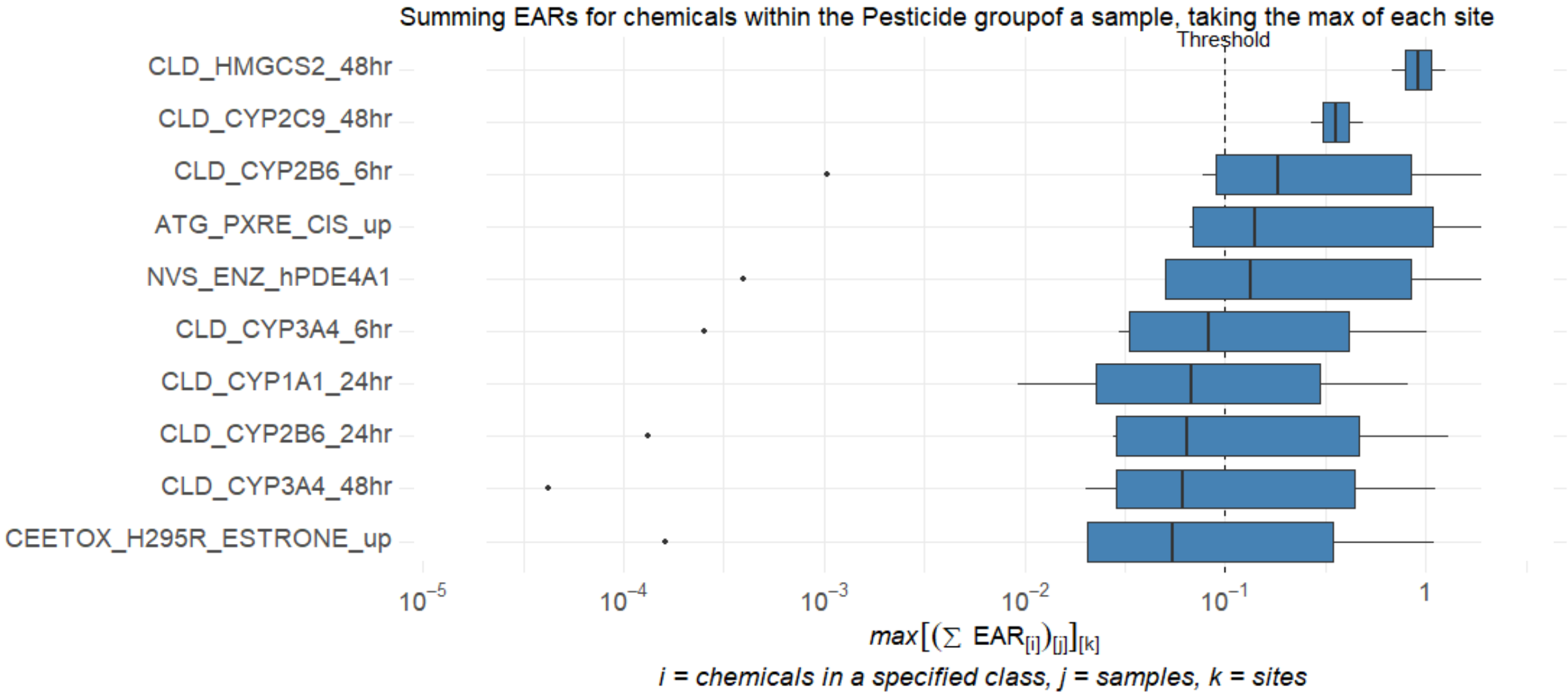
GRM, FMP, PBG all western main channel sites



Assays grouped by biological functionality



Pesticide class only activities affected



Xenobiotic metabolism highest EARs

Summary

- Maumee River AOC has a large agricultural influence
  - Site-specific urban and agricultural mixtures were identified
- Seasonal differences in flow and chemical use led to higher pesticides in June
- EARs revealed pesticides largely influenced biological activities associated with xenobiotic metabolism in the AOC
- Cluster Analysis and similar techniques may be an effective tool to characterize site and seasonal differences using chemical occurrence data
- Exposure-activity ratios can help prioritize contaminants and sites based on chemical potency and bioactivities affected

Questions?

Ankley GT.
Berninger, JP,
Blackwell B,
Cavallin JE,
Fay, KA,
Jensen KM,
Kahl MD,
Poole S,
Rearick, DC,
Randolph E,
Schroeder A,
Swintek, J,
Villeneuve DL

- Funding: Great Lakes Restoration Initiative (GLRI)
- - Grant to US EPA, US FWS, USGS

GENERAL DYNAMICS
Information Technology

Contact information:
Rearick.Daniel@epa.gov

Author information

- **Rearick, DC**[Δ]**,** Ankley GT[‡*]. Berninger, JP[‡], Blackwell B[‡], Cavallin JE[‡], Fay, KA[‡], Jensen KM[‡], Kahl MD[‡], Poole S[‡], Randolph E[‡], Schroeder A[†‡], Swintek, J[∞], Villeneuve DL[‡]
- [‡]U.S. Environmental Protection Agency, National Health and Environmental Effects Research Laboratory, Mid-Continent Ecology Division, Duluth, Minnesota, USA
- [†]University of Minnesota – Crookston, Math, Science, and Technology Department, Crookston, Minnesota, USA
- [Δ]General Dynamics, Information Technology, 6201 Congdon Blvd, Duluth, MN 55804
- [∞]Badger Technical Services, 6201 Congdon Blvd., Duluth, Minnesota 55804, United States