

Screening for biological relevance of environmental chemistry data using the toxEval software package

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Challenges of Assessing Environmental Monitoring Data

- Thousands of potential contaminants in the environment
 - Monitoring for hundreds per sample not uncommon
 - Improved analytical methods provide detections in the low ng/L
 - Difficult to determine what is of concern biologically

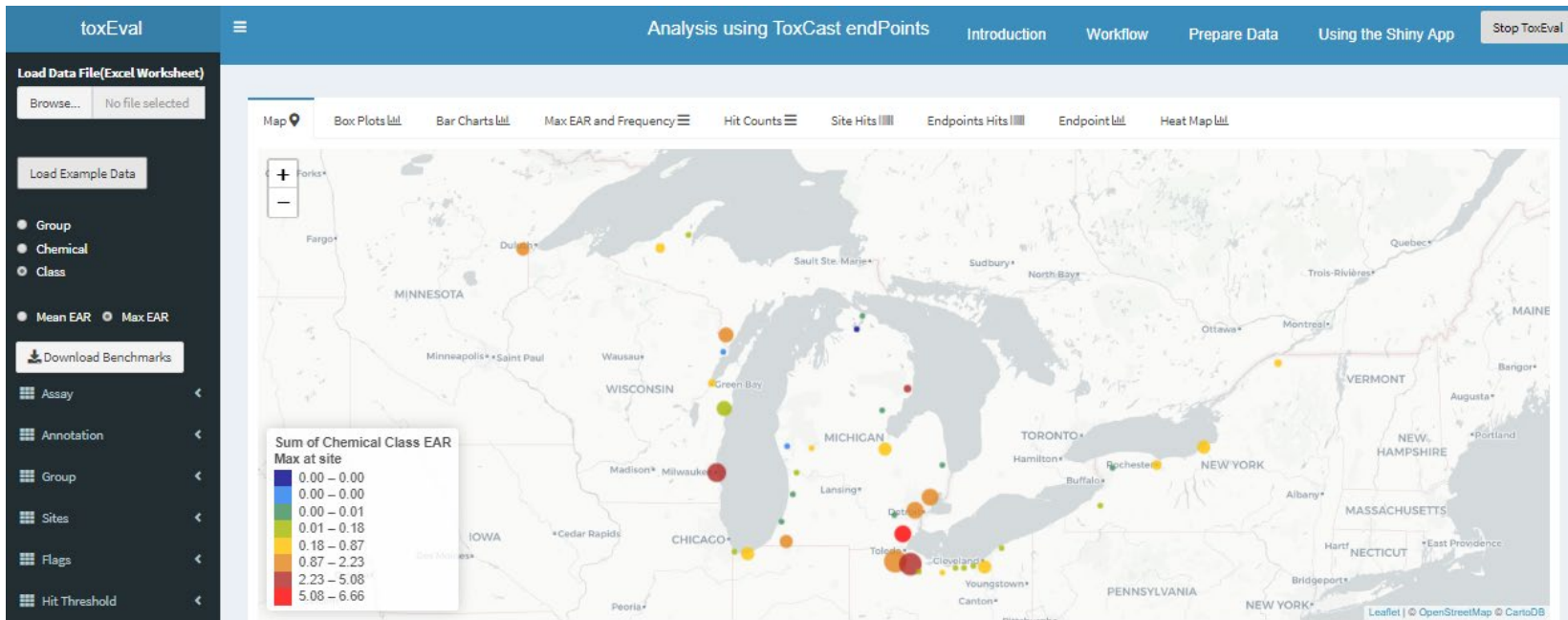
Needs:

- Prioritize chemicals, sites, and/or biological pathways
 - Provide stakeholders/decision makers with information to make informed decisions
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- ToxEval provides a tool for effects-based prioritization



Using toxEval for Prioritization

- ToxEval uses exposure:activity ratios (EARs) to prioritize based on the ToxCast database
 - >9000 chemicals screened through up to >300 assays
- Alternatively, toxEval can generate hazard quotients from user-provided benchmarks (aquatic life benchmarks, etc)
- Software package provides functions to analyze, visual, and organize concentration data based on selected endpoints



toxEval Analysis

ToxCast Endpoints:
Exposure-Activity
Ratio (EAR):

$$EAR = \frac{Concentration}{ACC}$$

Aquatic Life Benchmark
Hazard quotient (HQ):

$$HQ = \frac{Concentration}{Aquatic\ Life\ Benchmark}$$



Prioritize chemicals
and sites

Accessing toxEval

- Publicly available R package
 - Currently on GitHub
 - Download available through CRAN
- Intended audience:
 - Regulators and resource managers (federal, state, local)
 - Researchers (government, academia, industry, NGO)
- Current users: primarily government researchers



<https://github.com/USGS-R/toxEval>