Prioritization of Monitoring for Contaminants of Emerging Concern (CECs)

Stormwater Work Group

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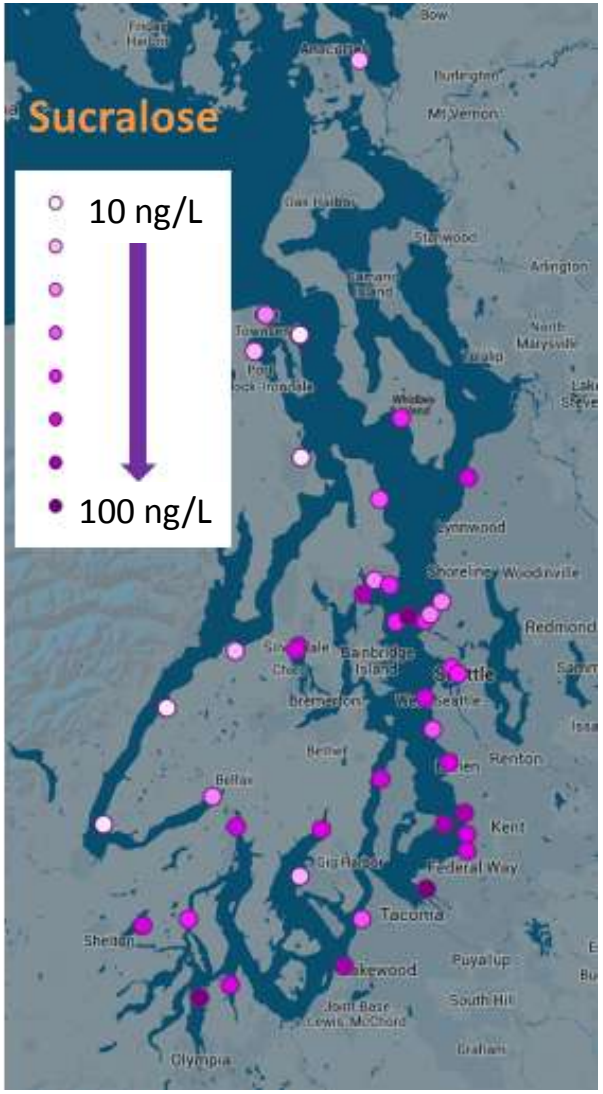
UNIVERSITY of WASHINGTON TACOMA

PUGET SOUND ECOSYSTEM MONITORING PROGRAM

Contaminants of Emerging Concern

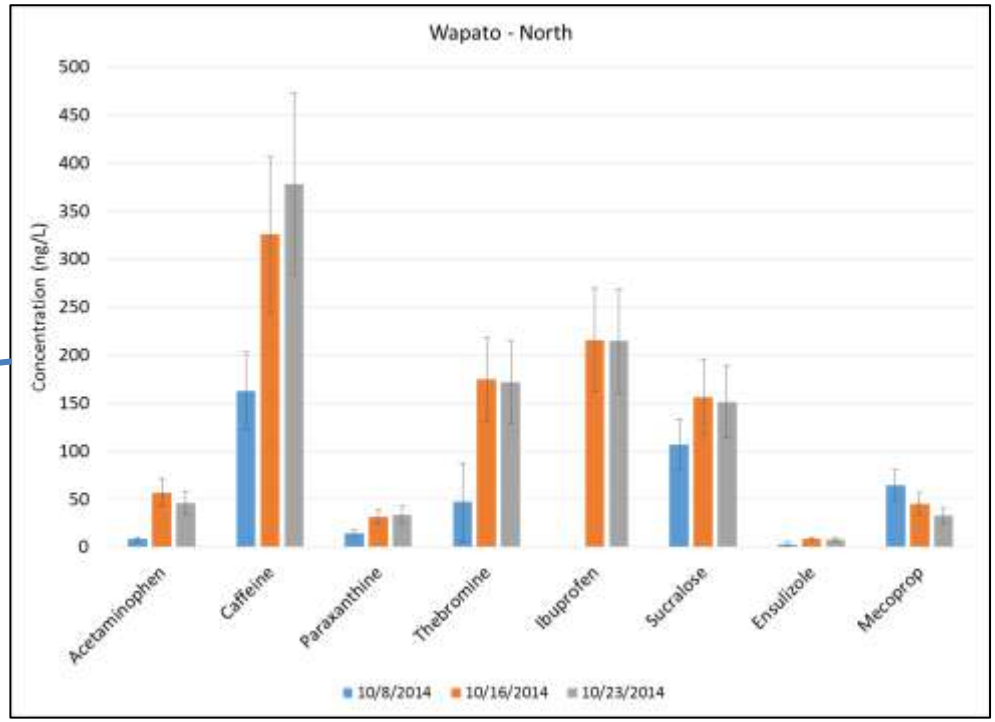
- No widely accepted definition of CECs. Generally:
  - Trace organics present at very low levels (µg/L or ng/L)
  - Previously unknown due to analytical limitations
  - Unregulated
  - May have biological impacts

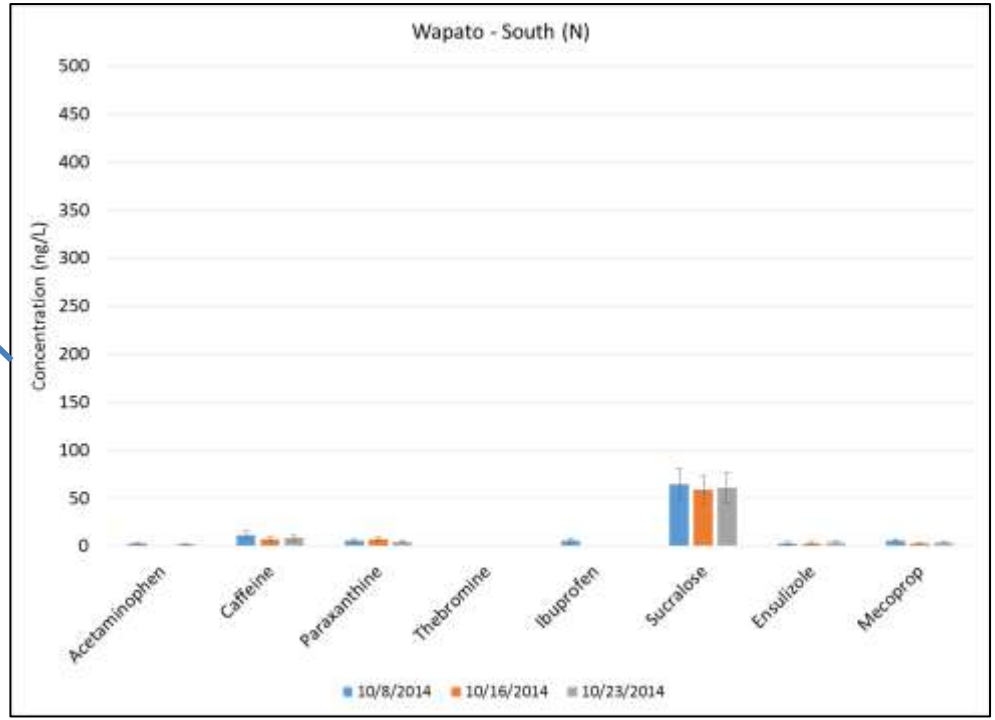


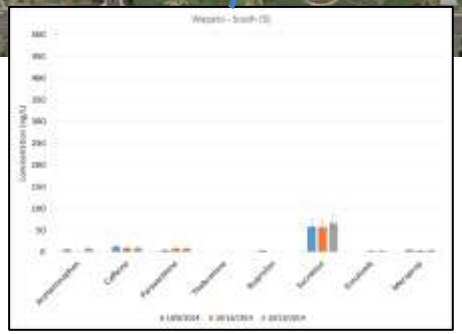
Miller-Schulze, 2014

Wapato Lake CEC Monitoring

Wapato Lake
Little Wapato Lake


Wapato - North
Concentration (ng/L)
500
450
400
350
300
250
200
150
100
50
0
Acetaminophen
Caffeine
Paraxanthine
Thebromine
Ibuprofen
Sucralose
Ensulizole
Mecoprop
10/8/2014
10/16/2014
10/23/2014


Wapato - South (N)
Concentration (ng/L)
500
450
400
350
300
250
200
150
100
50
0
Acetaminophen
Caffeine
Paraxanthine
Thebromine
Ibuprofen
Sucralose
Ensulizole
Mecoprop
10/8/2014
10/16/2014
10/23/2014



CEC Prioritization:

SUITE OF THOUSANDS OF POSSIBLE COMPOUNDS FOR CONSIDERATION. WHICH ARE THE MOST IMPORTANT TO MONITOR?

Challenges:

- Limited information on occurrence, variability, priority matrices, etc.
- Limited information on fate and transport
- Toxicity data are frequently absent or incomplete

from Schultz, 2014

Challenges of Prioritization: Data Limitations

Ranking method	No. of APIs	% of APIs
FPM	324	55.7
sold kg/year	397	68.2
PEC/PNEC	196	33.7
MEC_{SV}/PNEC	44	7.6
Cooper aq env	140	24.1
CEC	344	59.1
PBT	272	46.7
QSAR HQ	327	56.2
logP	580	99.7

FPM	Fish plasma model
PEC	Predicted environmental concentration
PNEC	Predicted no effect concentration
MEC	Measured environmental concentration
CEC	Critical environmental concentration
PBT	Persistency, bioaccumulation, toxicity
QSAR	Quantitative structure-activity relationship
HQ	Hazard quotient

Number and percentage of Active Pharmaceutical Ingredients in the prioritisation database (total: 582) that could be ranked according to nine different prioritisation schemes.

Roos, V.; Gunnarsson, L.; Fick, J.; Larsson, D. G. J.; Ruden, C., Prioritising pharmaceuticals for environmental risk assessment: Towards adequate and feasible first-tier selection. *Science of the Total Environment* **2012,** *421*, 102-110.

CEC Prioritization:

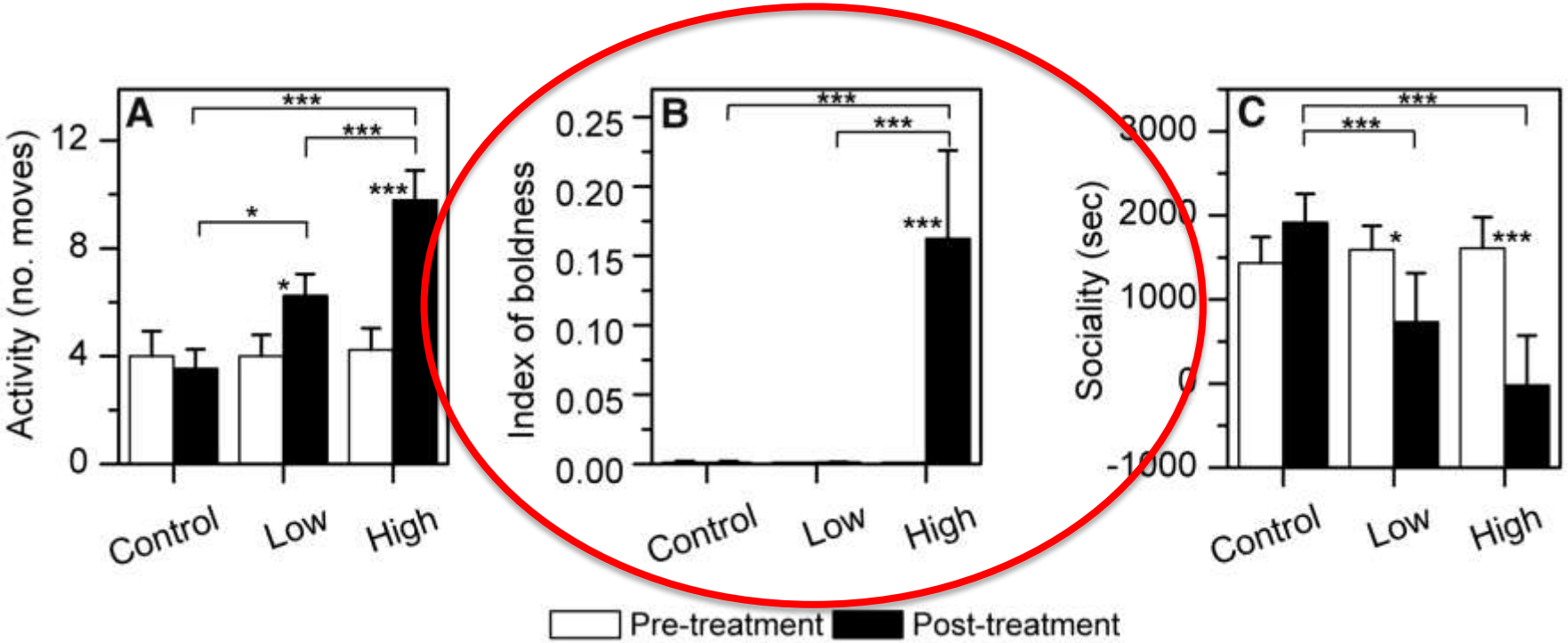
SUITE OF THOUSANDS OF POSSIBLE COMPOUNDS FOR CONSIDERATION. WHICH ARE THE MOST IMPORTANT TO MONITOR?

Challenges:

- Limited information on occurrence, variability, priority matrices, etc.
- Limited information on fate and transport
- Toxicity data are frequently absent or incomplete
- Not generally a lethality risk
  - Concerns are for sub-lethal effects impacting growth, reproduction, development

from Schultz, 2014

Challenges of Prioritization: Biological Impacts



Fish (European perch) behavioral response to two concentrations (low: 1.8 μg L^{-1}; high: 910 μg L^{-1}) of dissolved oxazepam compared to control (0 μg L^{-1}).(**A**) **Activity,** measured as number of swimming bouts (>2.5 cm) during 10 min. (**B**) **Boldness**, measured as the inverse of latency to enter a novel area during the total trial time (900 s). (**C**) **Sociality**, measured as the cumulative time (in seconds) spent close to a group of conspecifics. Error bars represent ±1 SE (n = 25 in all treatments); statistically significant differences between the pre- and posttreatments are indicated (*P < 0.05 or ***P < 0.001).

Published by AAAS

T Brodin et al. Science 2013;339:814-815

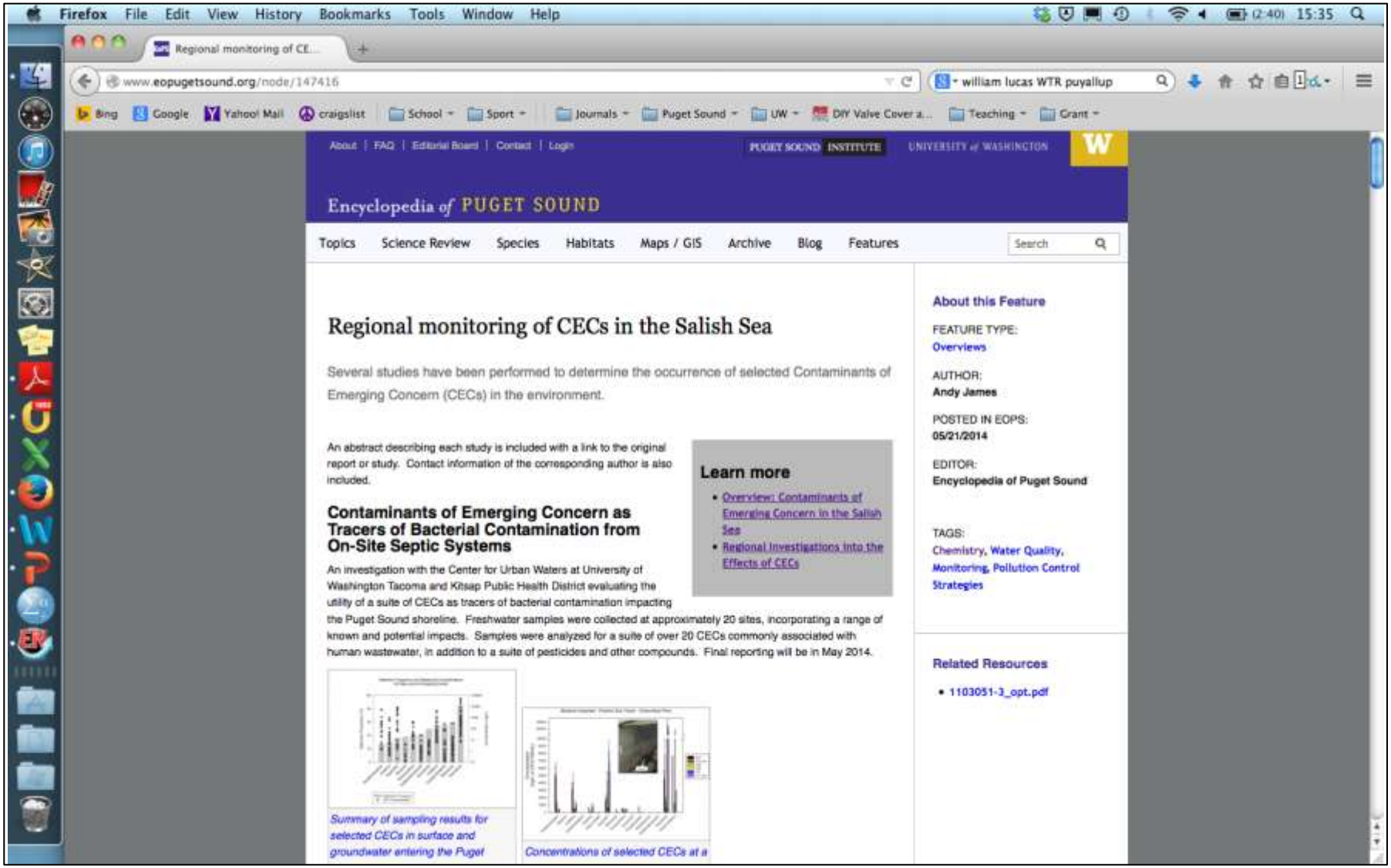
Science
AAAS

CEC Prioritization Framework: PSEMP White Paper

Objective: Develop a process to prioritize monitoring of CECs in the environment

1. Literature Review
   - Other prioritization processes and regional monitoring data

Regional CEC Investigations: Encyclopedia of Puget Sound



CEC Prioritization Framework: PSEMP White Paper

Objective: Develop a process to prioritize monitoring of CECs in the environment

1. Literature Review
   - Other prioritization processes and regional monitoring data
2. Conceptual Exposure Models
   - Pressure framework (what are likely sources?)
   - Exposure framework (fate and transport?)

CEC Prioritization Framework: PSEMP White Paper

3. Define Prioritization Process

Many potential approaches and considerations
The approach can impact the outcome.

- usage
- occurrence
- persistence
- bioaccumulation
- toxicity/sublethal impacts
- human exposure
- available data
- status of analytical methods
- costs
- programmatic concerns
- opportunities for reduction

Comparison of Prioritization Schemes

- Decision points impact the final list of priority CECs.

Table 4-3. High Priority TOrCs Obtained from Each of the Three Prioritization Approaches.

Approach #1	Approach #2	Approach #3
Coprostanol	Pentachlorophenol	3-methylcholanthrene
17α-ethynylestradiol	PBDE-209	o,p'-DDE
Cholesterol	Tonalide	Mirex
Stigmastanol	Galaxolide	p,p'-DDE
β-sitosterol	Tamoxifen	cis-Nonachlor
Stigmasterol	Hexabromocyclododecane	p,p'-DDT
17β-estradiol	Desmosterol	p,p'-DDD
Bis(2-ethylhexyl)adipate	Cholesterol	o,p'-DDT
PBDE-209	Epicoprostanol	trans-Nonachlor
Bis(2-ethylhexyl)phthalate	Coprostanol	γ-Chlordane
Mestranol	Campesterol	trans-Chlordane
Di-N-octyl phthalate	Stigmasterol	Trifluralin
Desmosterol	β-sitosterol	Ethalfluralin
Cholestanol	Stigmastanol	Benfluralin
4-Nonylphenol	cis-Chlordane	PBDE-209
4-n-nonylphenol	Bis(2-ethylhexyl)adipate	Miconazole
Estrone	4-nonylphenol diethoxycarboxylate	cis-Chlordane
Testosterone	4-nonylphenol monoethoxylate	pentachloro-Benzenethiol
Novobiocin	4-Nonylphenol	3-chloro-2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-Benzenamine
Campesterol	4-n-nonylphenol	Aldrin

CEC Prioritization Framework: PSEMP White Paper

3. Define Prioritization Process

- Risk based approach
  - Most important compounds are those which may result in biological impacts
  - Prioritize by comparing measure of occurrence with measure of impact
  - Priority compounds may also include those with high potential solely based on toxicity data
- Include consideration of data limitations
  - Group compounds into “management” categories based on availability of occurrence and toxicity data.
  - Categories include next-steps for each group.

CEC Prioritization Framework: PSEMP White Paper

3. Define Prioritization Process (cont.)

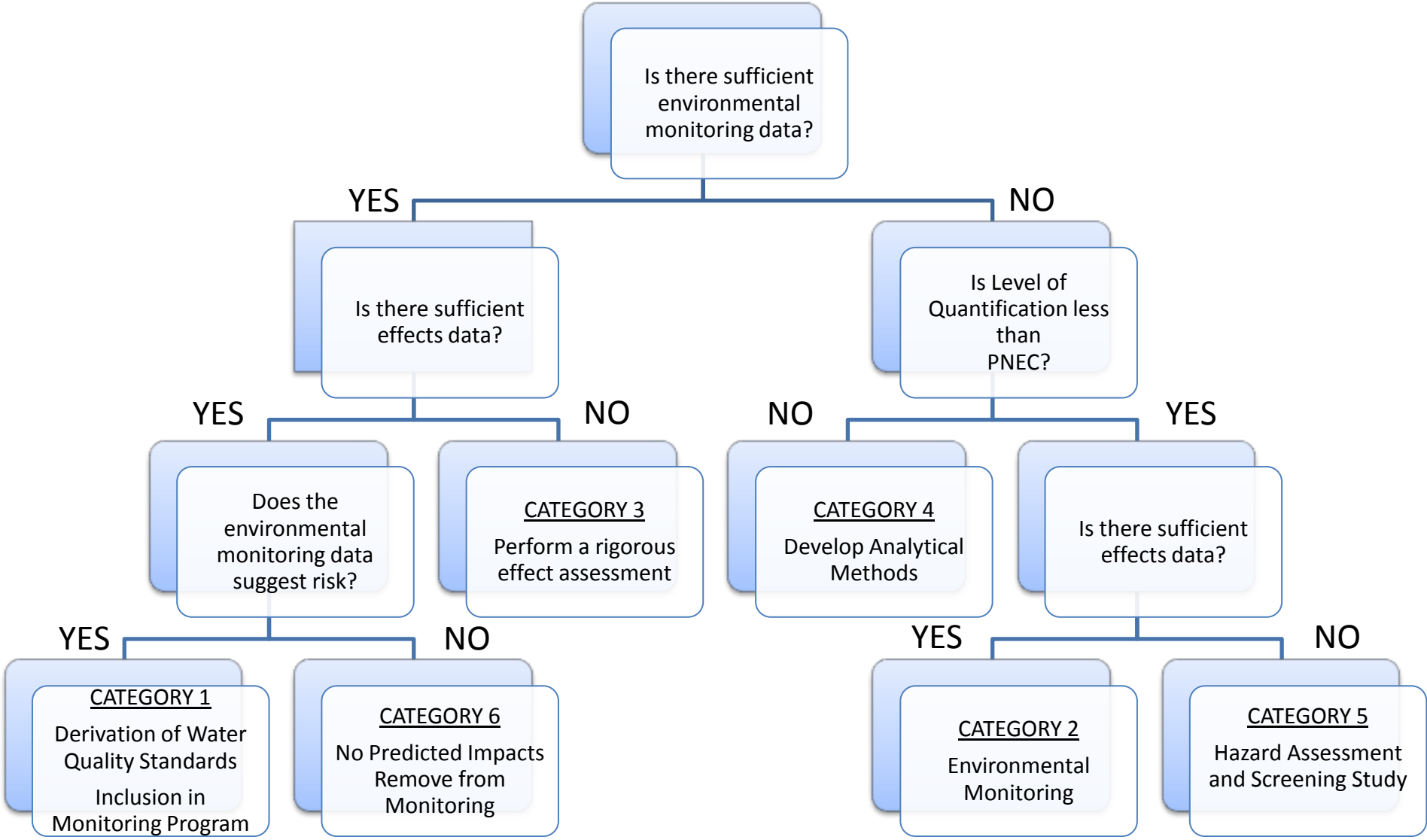
- Include Consideration of Biological Endpoints
  - There may be observed biological responses without identified causative agents
  - Based on exposure-response and Adverse Outcome Pathway research, information about effect may be useful in identifying an associated compound or class of compounds, which can then focus monitoring efforts.
  - Biological endpoint monitoring can inform on the status and/or changes in environmental condition.

CEC Prioritization Framework

Illustrative Example of Prioritization Framework

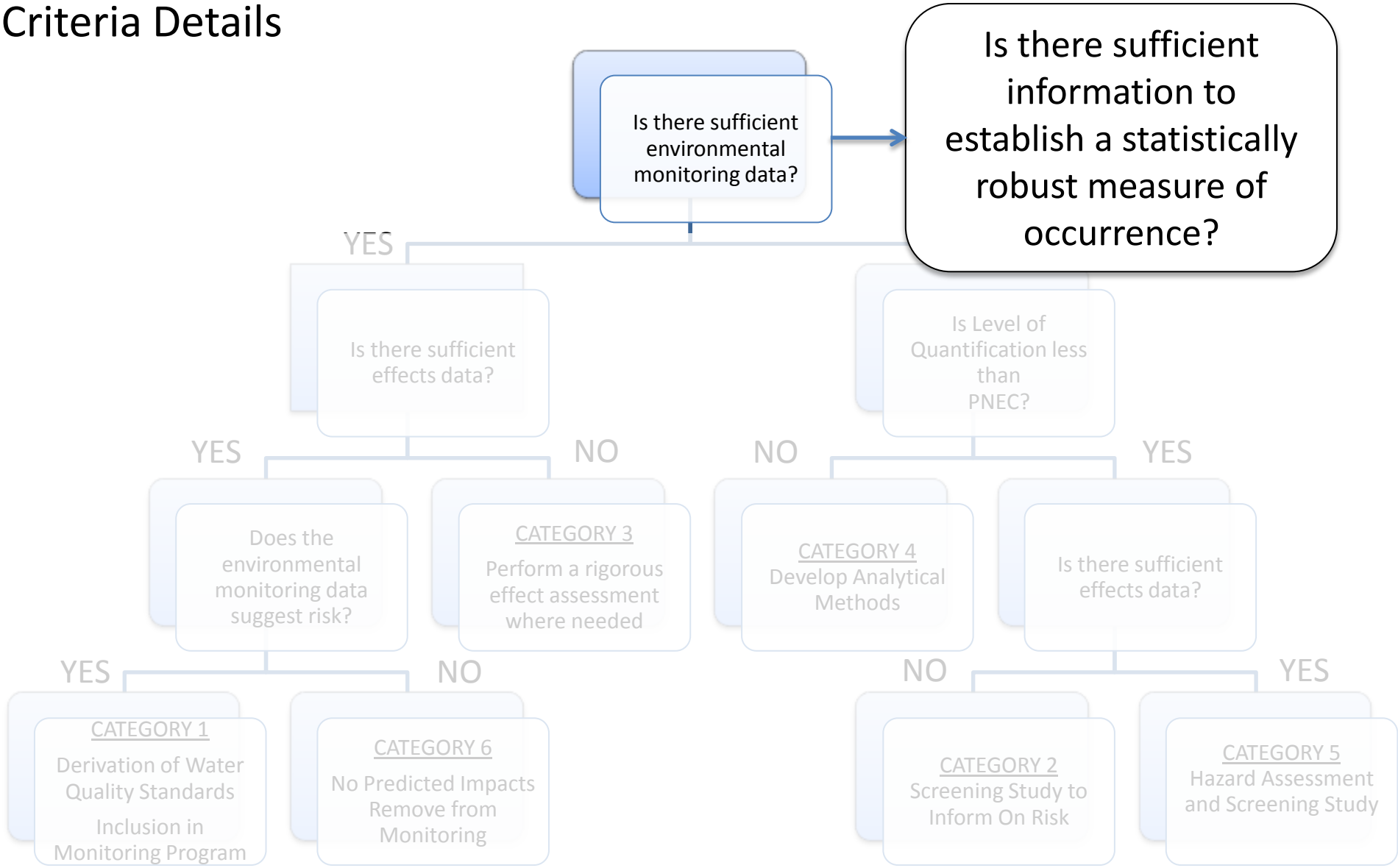
1. Categorize compounds based on available information
2. Rank compounds utilizing a risk-based approach

Step 1:
CATEGORIZE COMPOUNDS



Adapted from von der Ohe et al (2011) *Sci of the Total Envr*, *409*, 2064-2077.

STEP 1: CATEGORIZE COMPOUNDS
Criteria Details



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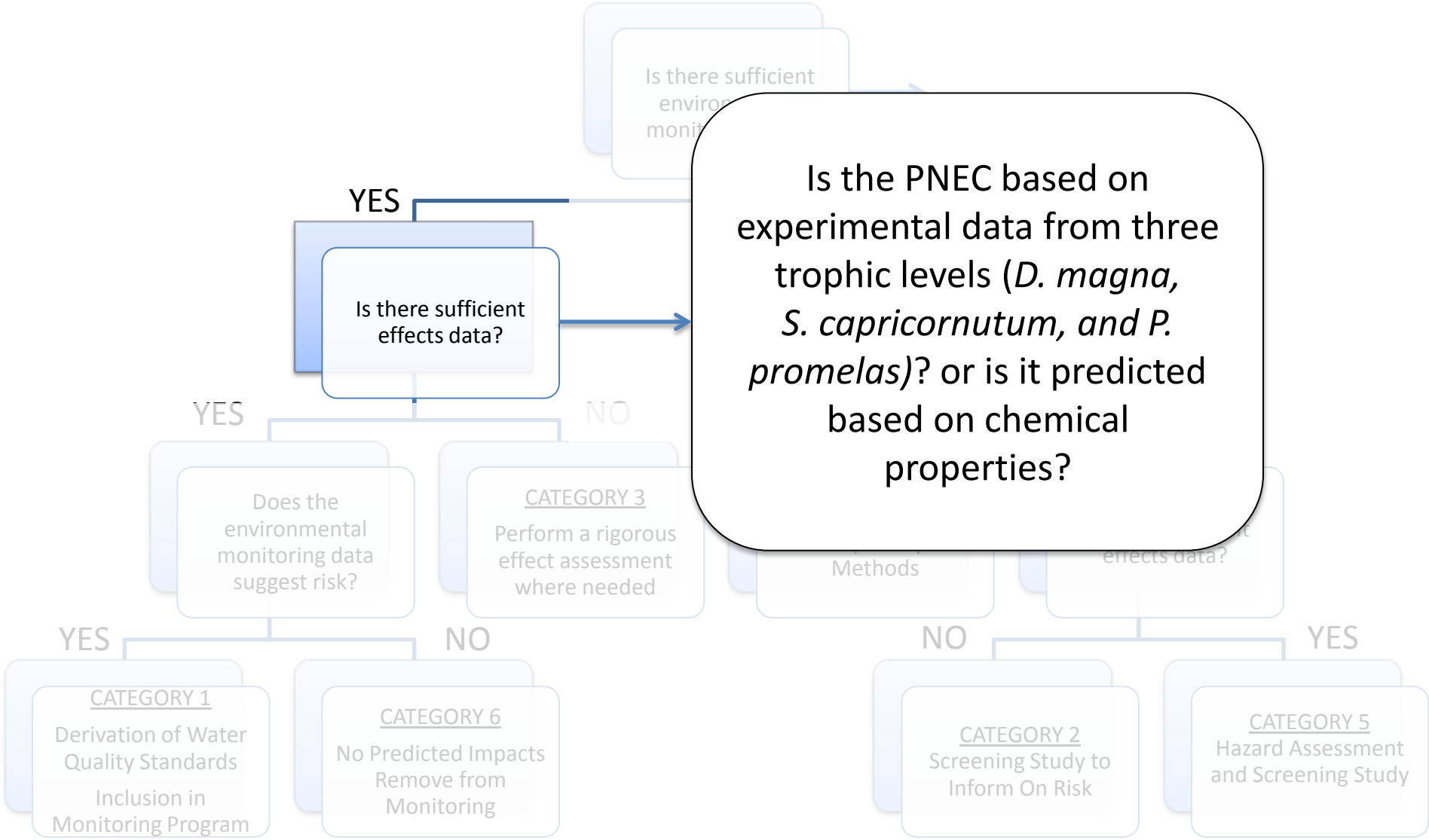

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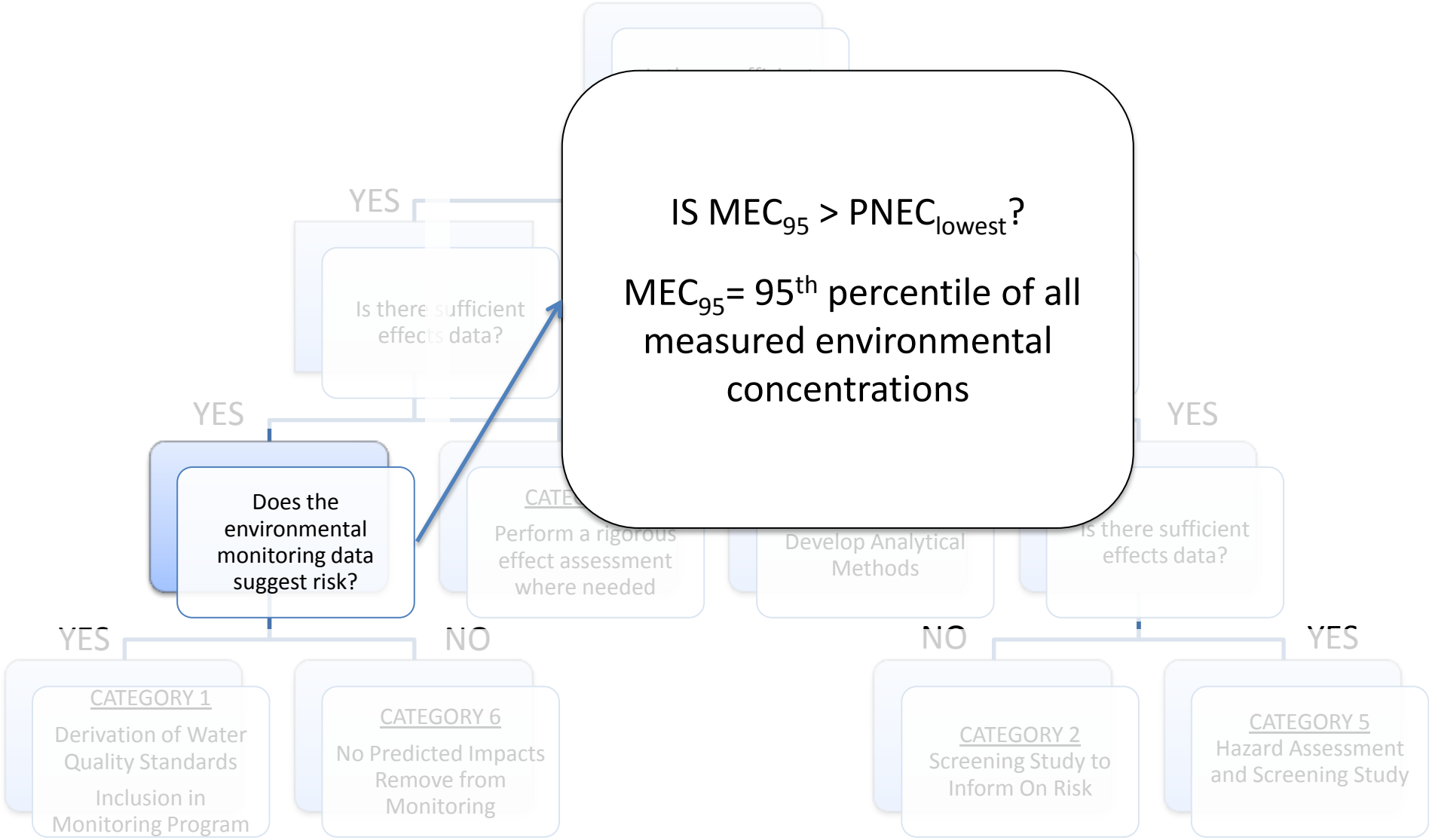
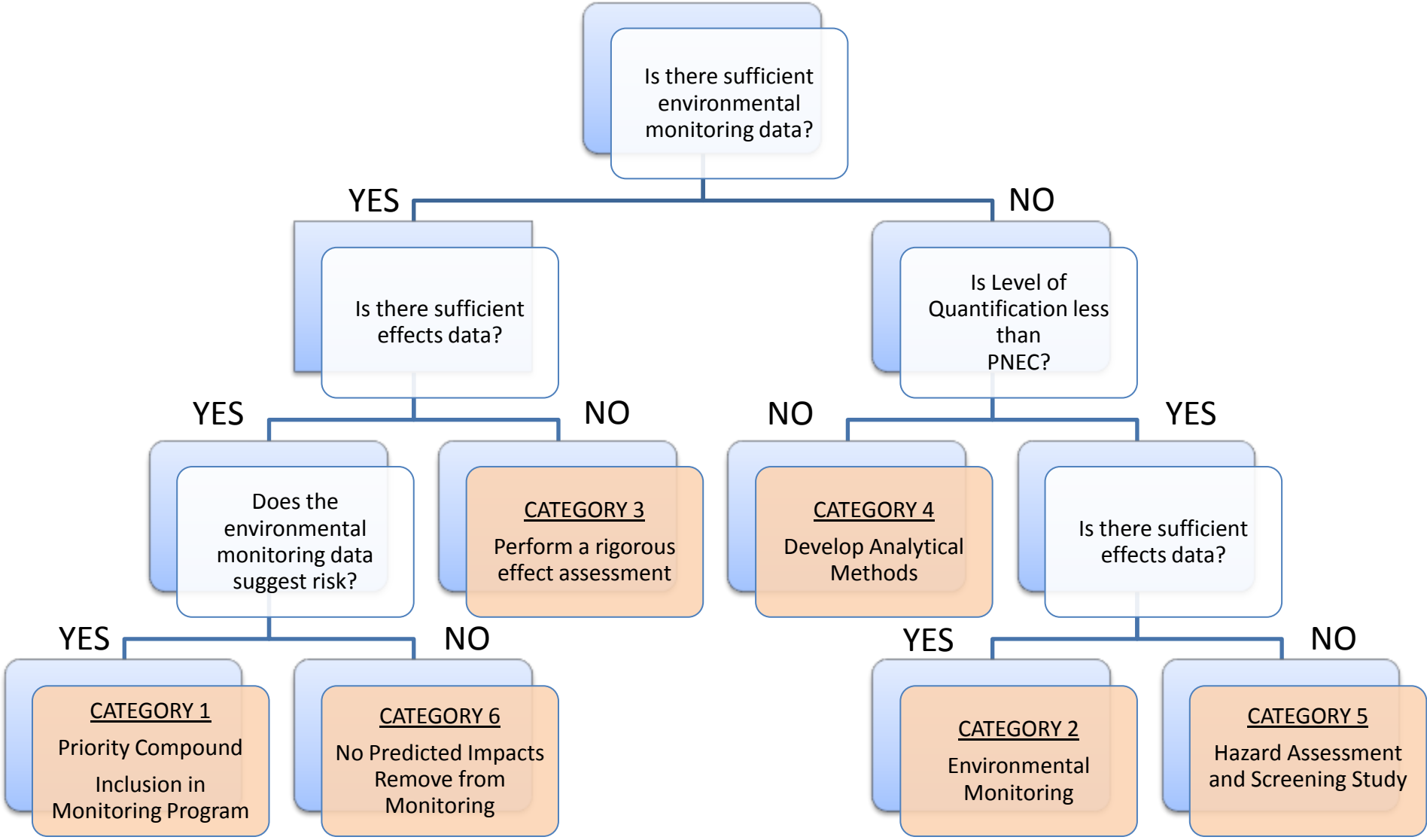


STEP 1: CATEGORIZE COMPOUNDS

Categories Determine Next Steps



Adapted from von der Ohe et al (2011) *Sci of the Total Envr*, *409*, 2064-2077.

Step 2: PRIORTIZATION WITHIN CATEGORIES

Priority Compounds

Priority compounds are those where measured value is greater than effects levels e.g., MEC_{95}>PNEC

Also include those compounds with low effects levels e.g., PNEC < 0.1 µg/L

MEC - Measured Environmental Concentration
PNEC - Predicted No Effects Level

CEC Prioritization Framework: PSEMP White Paper

4. Other important factors

- Include method for reevaluating CECs list based on new and/or revised information
  - New data on effects or biological responses
  - Introduction (or removal) of pharmaceuticals
- Method should include stakeholder engagement and review. Currently being performed by PSEMP in conjunction with Columbia River Toxics Reduction group (EPA and USGS)

PSEMP CEC Prioritization: Next Steps

- White paper is complete
- Developing a case study to inform on issue (finalize January 2015)
- Reconvene to develop strategy for implementation

THANK YOU

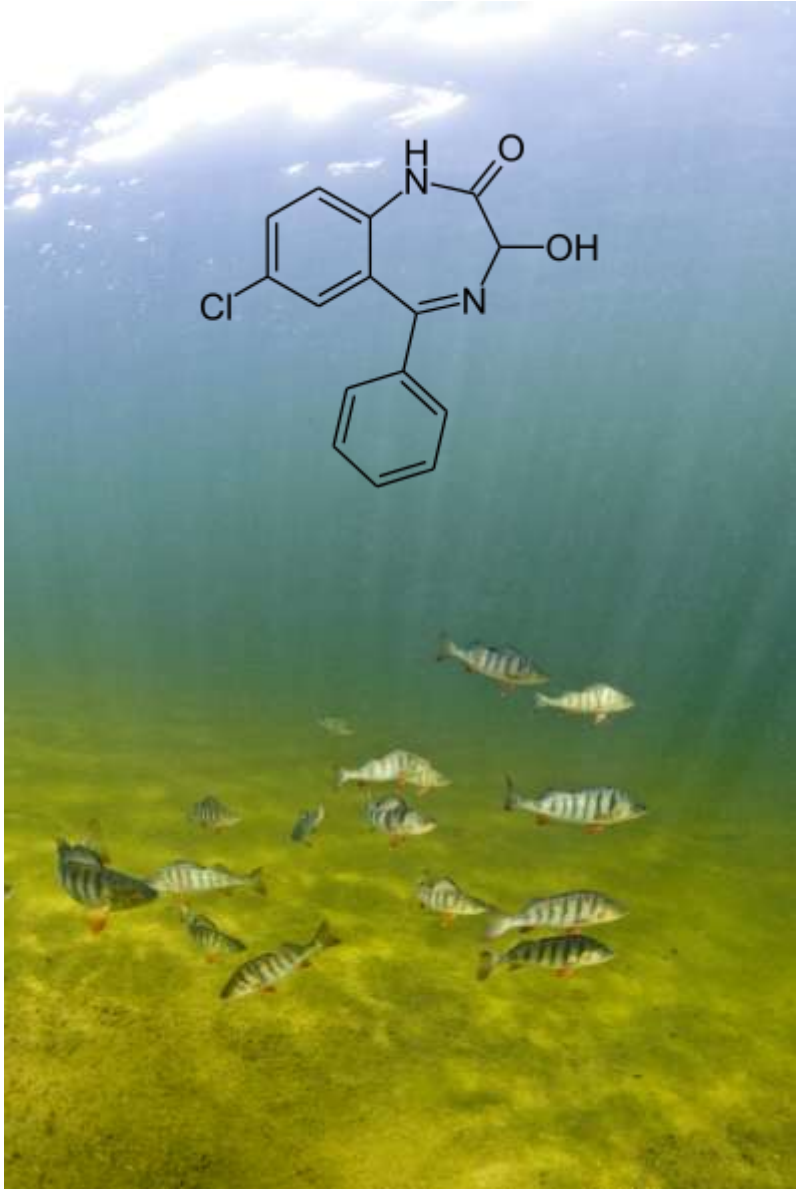
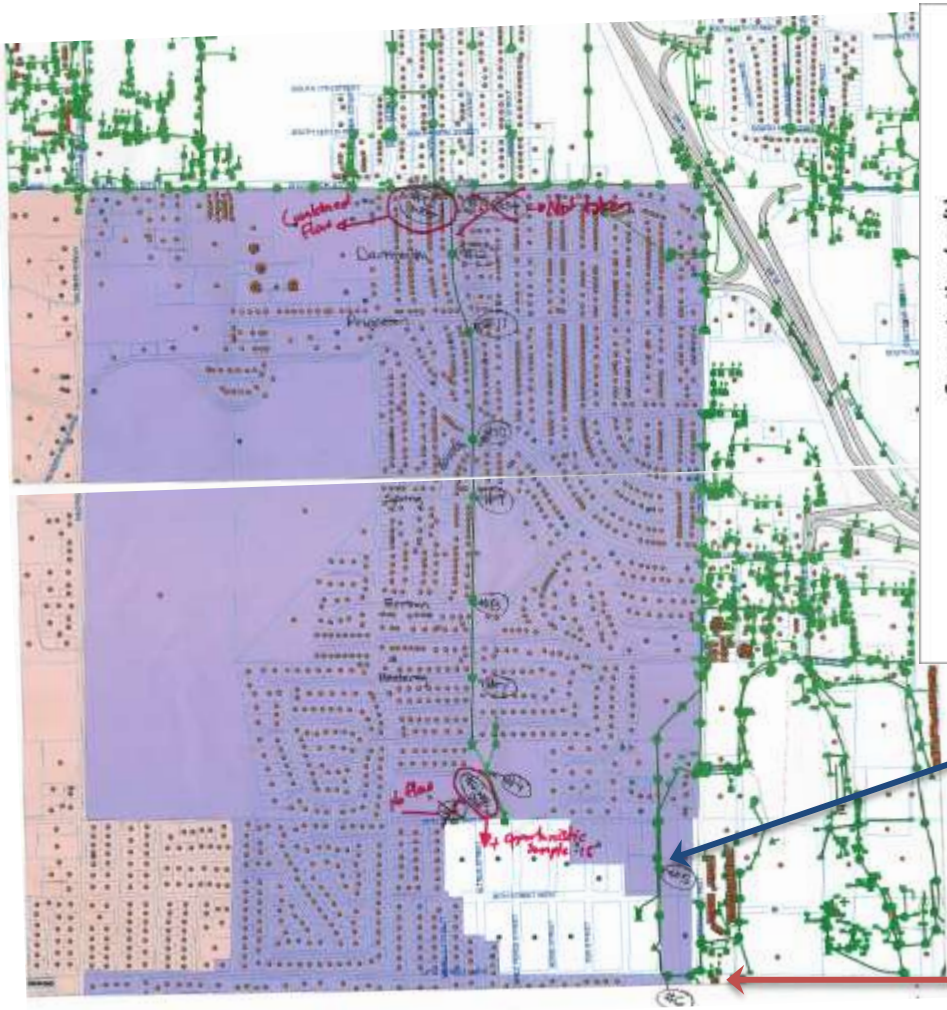
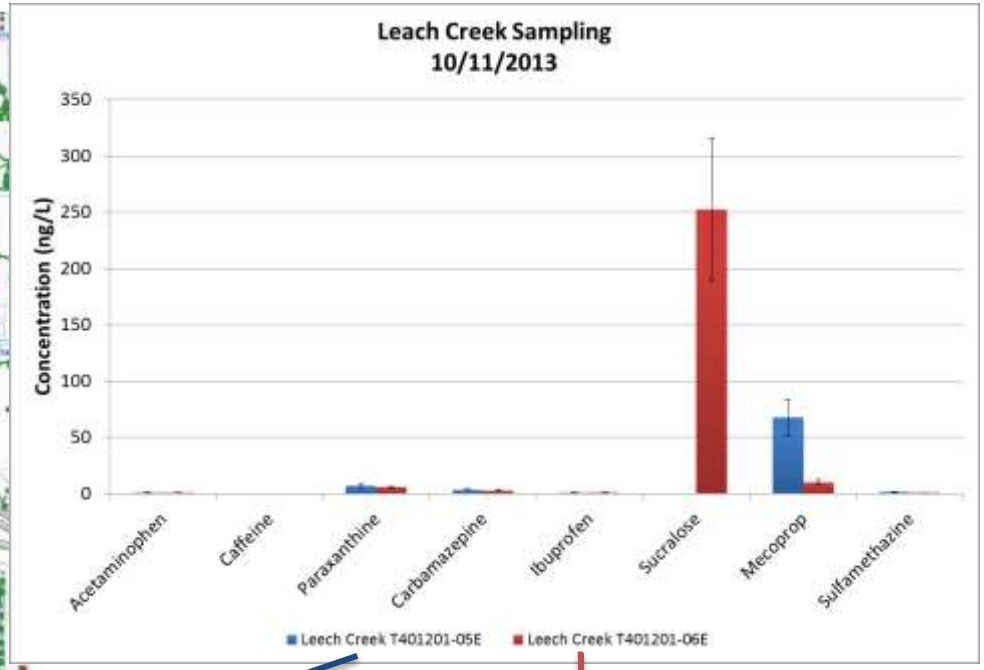


Photo: Johan Gunséus

Stormwater Conveyance System Sampling
Leach Creek





CEC Prioritization Framework: PSEMP White Paper

3. Define Prioritization Process

- **What chemical characteristics are important to prioritization**
  - usage
  - occurrence
  - persistence
  - bioaccumulation
  - toxicity/sublethal impacts
  - human exposure

- **How are the criteria determined**
  - toxicity - QSAR (e.g., ECOSAR) or through experimental data. What threshold?
  - sublethal effects?
  - mixture effects?
  - occurrence – predicted or measured environmental concentration

CEC Prioritization Framework: PSEMP White Paper

3. Define Prioritization Process

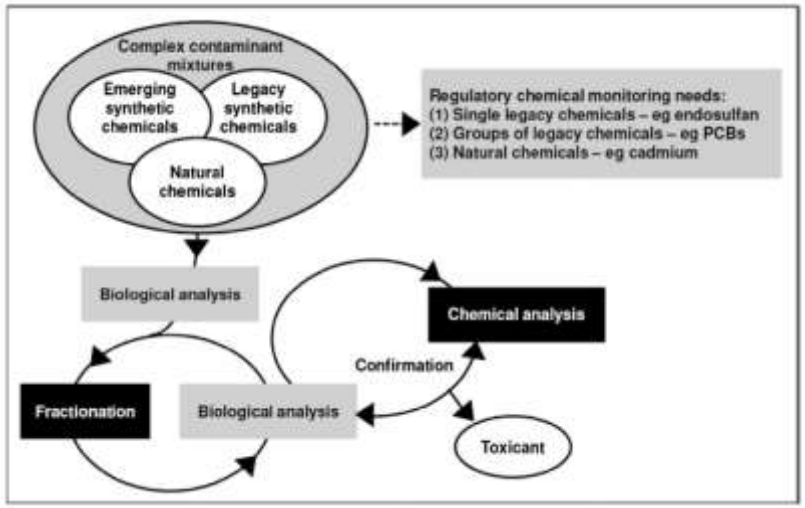
- **Other factors important in the prioritization process**
  - available data
  - status of analytical methods
  - analytical capabilities
  - costs
  - programmatic concerns
  - opportunities for reduction

- **Define how are the criteria/properties applied**
  - screening (e.g., any compound with a BCF < 5000 will be ignored; t½>7days ➔ persistent)
  - weighting
  - risk based
  - hazard based
  - extent of exceedance over threshold value

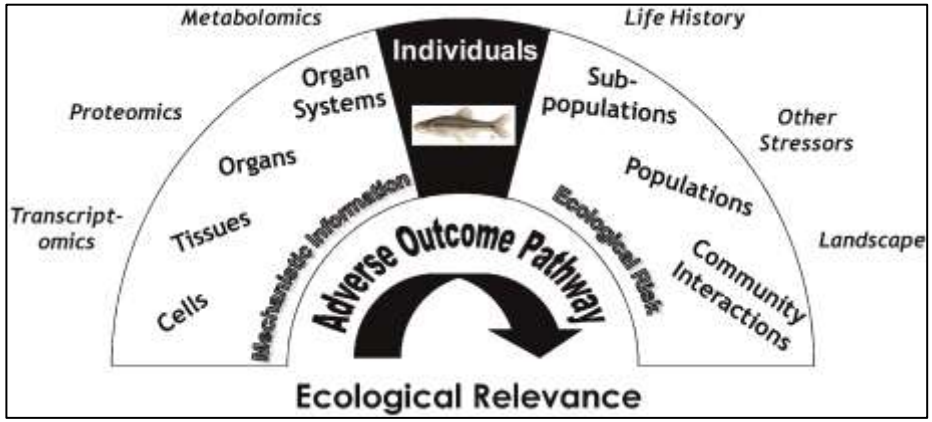
CEC Prioritization Framework: PSEMP White Paper

3. Define Prioritization Process

- **How to incorporate measures of biological endpoints?**



Schematic of biological effects-directed analysis with chemical monitoring to focus investigation and identification of priority chemicals (Hutchinson et al. 2013)



Adverse outcome pathways (AOPs) relating individual organisms to ecologically relevant levels of biological organization (Kramer et al. 2011)