A Framework for Prioritizing Chemicals in Retrospective Ecological Assessments: Application to a Great Lakes Watershed

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Background

- Anthropogenic activities have resulted in the frequent detection of **contaminants of emerging concern** (CECs) in inland and coastal watersheds (e.g., Baldwin et al. 2020; Elliot et al., 2017; Glassmeyer et al., 2017; Kiesling et al., 2019; Peng et al., 2018).
- Due to the large number of detected CECs and the often limited amount of resources available for risk assessment and/or regulation there is often the need for **chemical prioritization**.
- **New approach methodologies** (NAMs) provide novel tools, techniques, and data that can be employed to supplement traditional datasets for risk-based prioritization of CECs (Ankley et al., 2021; Blackwell et al., 2017; Cavallin et al., 2021; Corsi et al., 2019; Ekman et al., 2013; Li et al., 2017).

Aim: Describe an alternative chemical prioritization framework incorporating <u>both</u> traditional and newer approach methodologies, and demonstrate its application using data from caged-fish studies carried out in the Milwaukee Estuary (2017 – 2018) **(Presentation # 01.05.16).**

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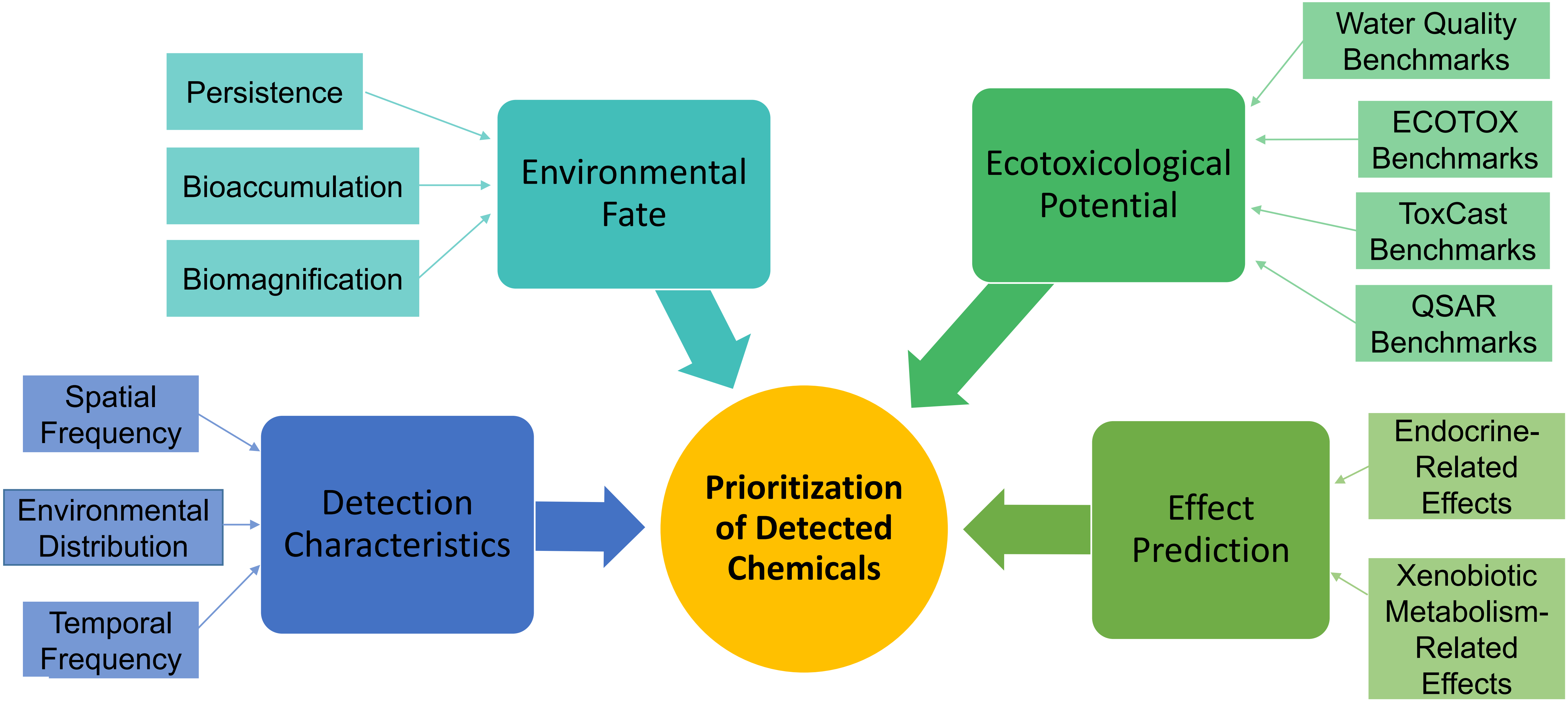
Weight-of-Evidence Prioritization Framework



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Chemical Prioritization

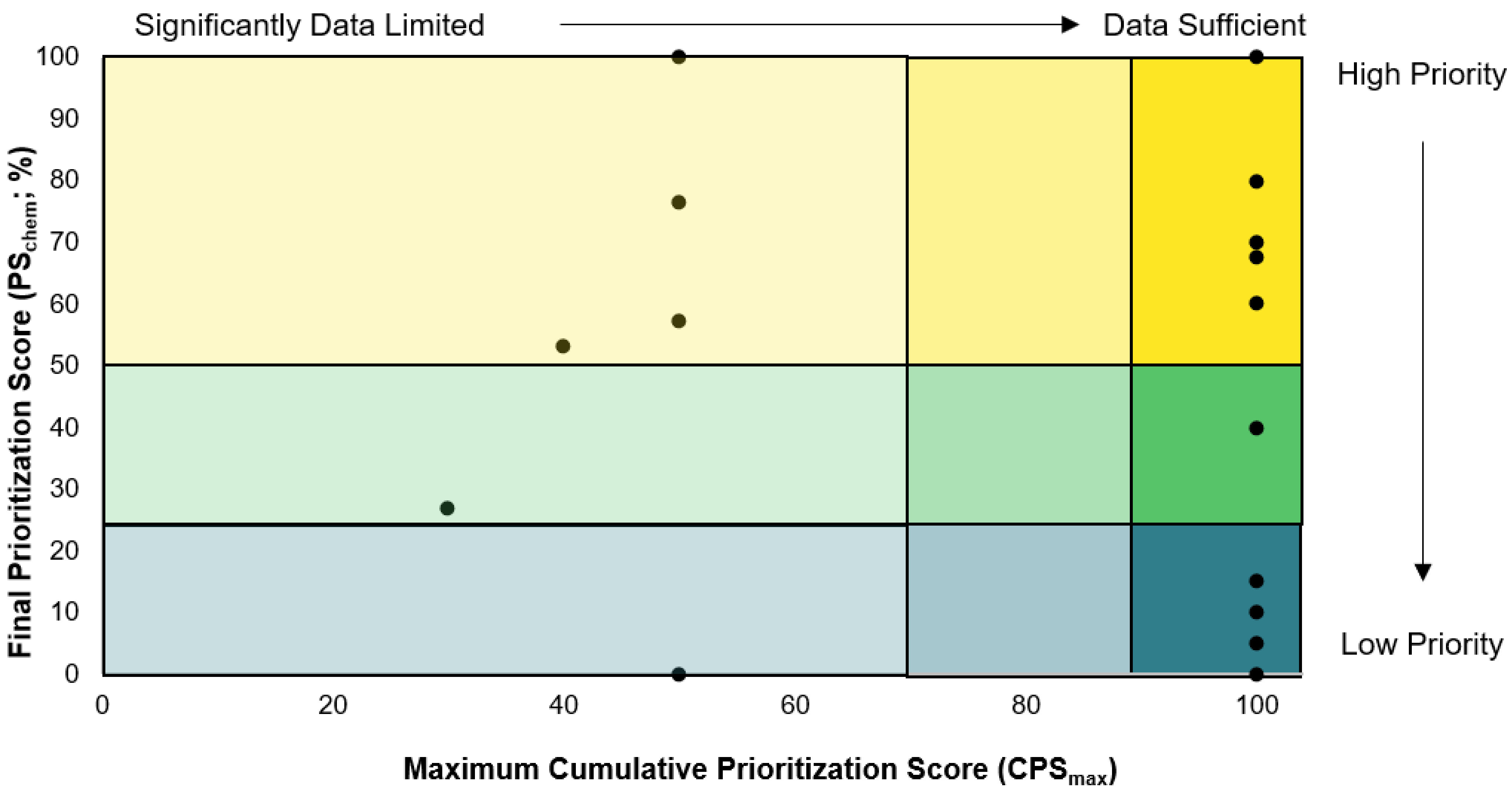
Chemical	Detection Characteristics			Environmental Fate			Ecotoxicological Potential				Effect Prediction			
	Spatial Frequency	Temporal Frequency	Environmental Distribution	Persistence	Bioaccumulation	Biomagnification	Water Quality Benchmark	ECOTOX Benchmark	ToxCast Benchmark	QSAR Benchmark	Endocrine-Related	Xenobiotic-Metabolism Related	CPS	PS_{chem} (%)
XX-XX-X	10	10	10	10	10	10	15	10	5	5	2.5	2.5	100	**100**
	10	10	10	10	10	10	DL	DL	DL	DL	2.5	2.5	65	**100**
	10	10	0	10	10	10	5	10	5	5	2.5	2.5	80	**80**
	10	5	5	10	5	5	DL	10	5	5	2.5	2.5	65	**76.5**
	10	5	5	10	5	5	5	10	5	5	2.5	2.5	70	**70**
	10	5	5	10	5	5	2.5	10	5	5	2.5	2.5	67.5	**67.5**
	5	5	5	5	10	5	5	5	5	5	2.5	2.5	60	**60**
	5	5	5	5	5	5	DL	DL	DL	5	2.5	2.5	35	**57.1**
	5	5	5	10	5	5	DL	5	DL	DL	1.25	0	41.3	**55**
	5	0	10	0	5	5	0	5	5	5	0	2.5	42.5	**42.5**
	5	5	5	0	0	0	DL	DL	0	0	0	2.5	17.5	**23.3**
	0	5	5	0	0	0	0	0	0	0	1.25	1.25	12.5	**12.5**
	5	0	5	0	0	0	0	0	0	0	0	0	10	**10**
	0	0	0	0	0	0	0	0	0	0	0	2.5	2.5	**2.5**
	0	0	0	0	0	0	DL	DL	DL	DL	0	0	0	**0**
XX-XX-X	0	0	0	0	0	0	0	0	0	0	0	0	0	**0**

Prioritization Score (PS)

High ← Low 0 DL

$$PS_{chemical}\ (\%) = \frac{\Sigma PS_{detect} + \sum PS_{fate} + \sum PS_{benchmark} + \sum PS_{effect}}{CPS_{max}}\ x\ 100$$

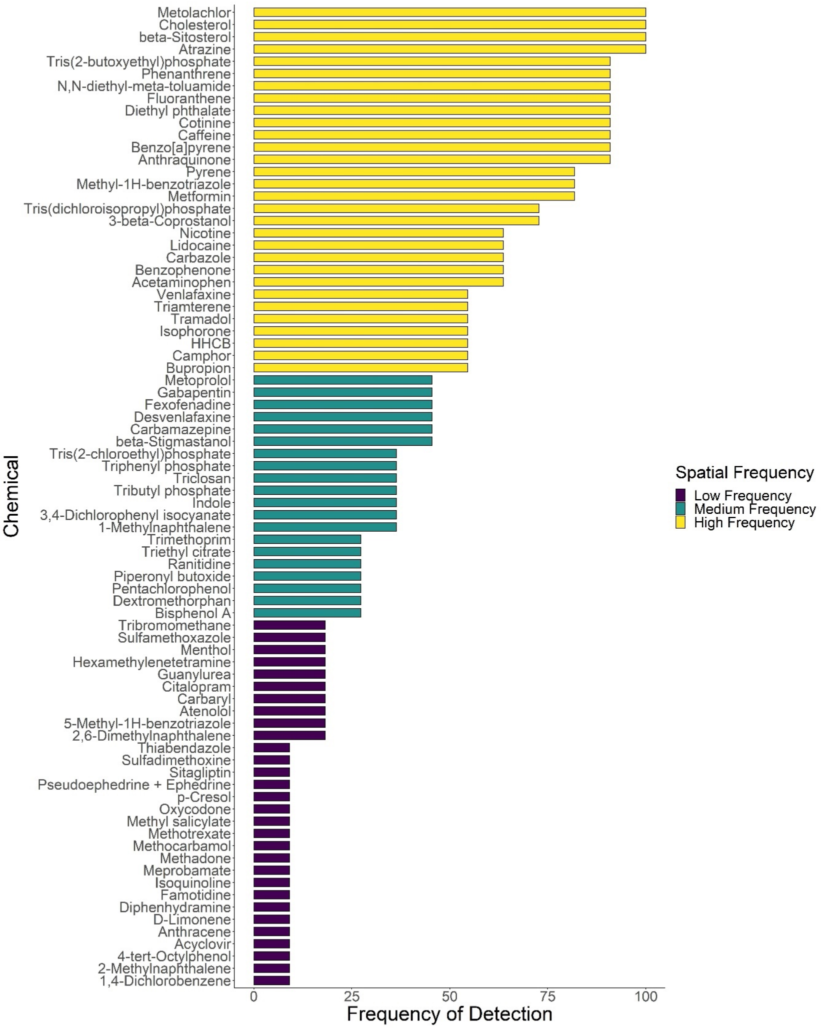
Chemical Prioritization



Detection Characteristics

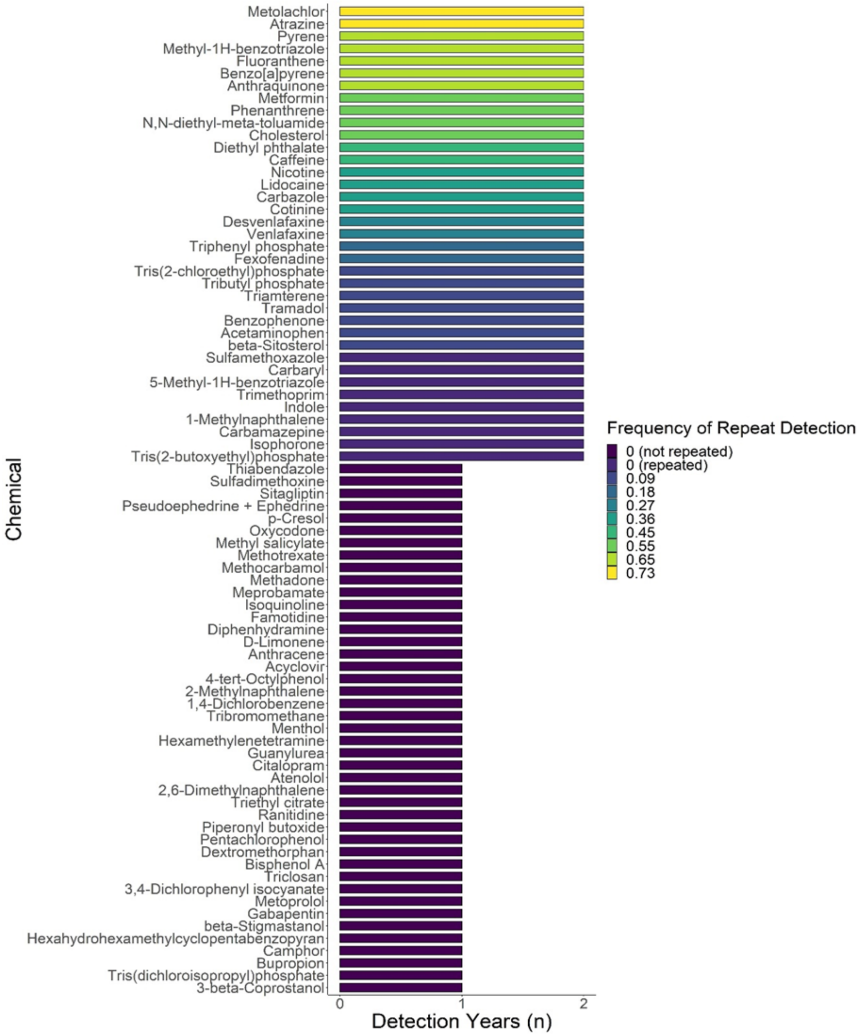
PS = 0 - 10

Spatial Frequency



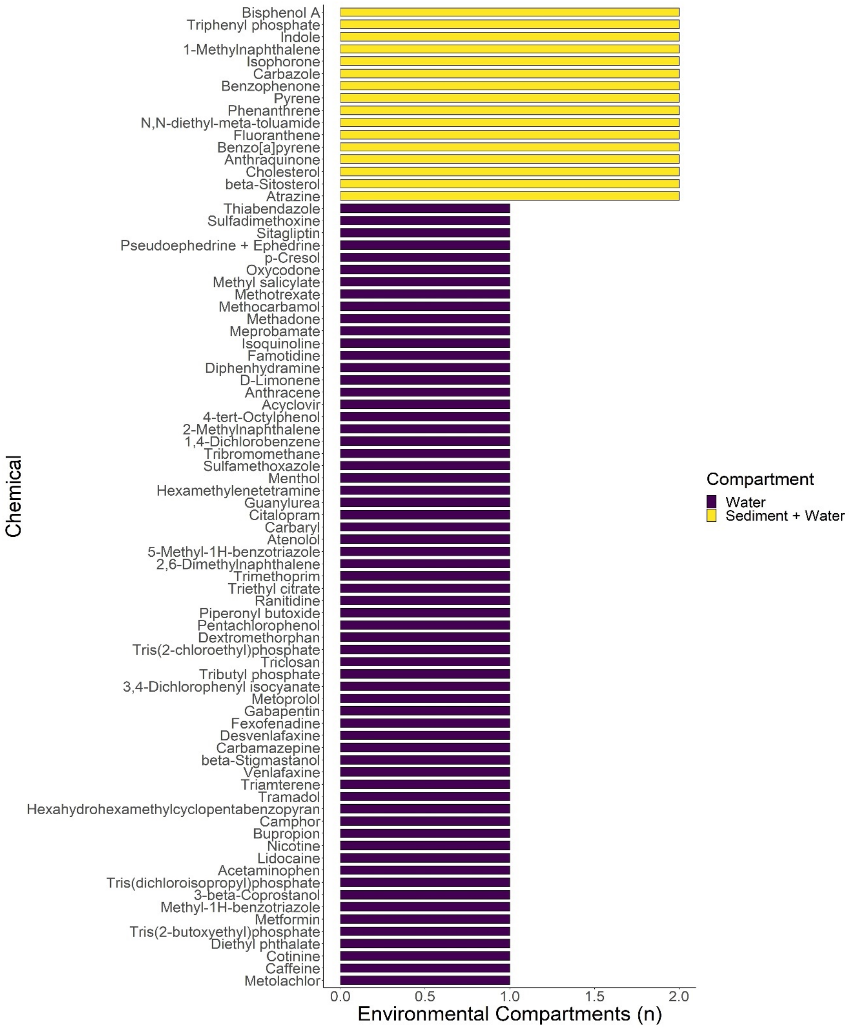
Frequency of detection across sites.

Temporal Frequency



Frequency of detection across years.

Environmental Distribution



Number of detect compartments.

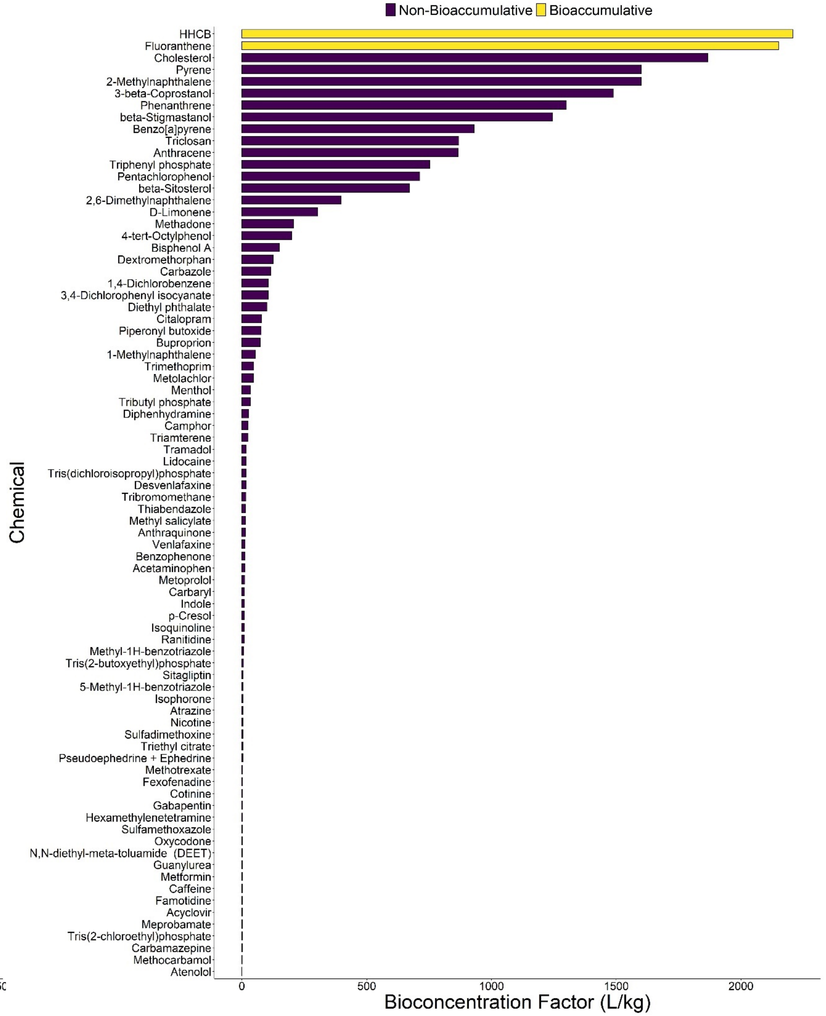
Environmental Fate

PS = 0 - 10

Persistence

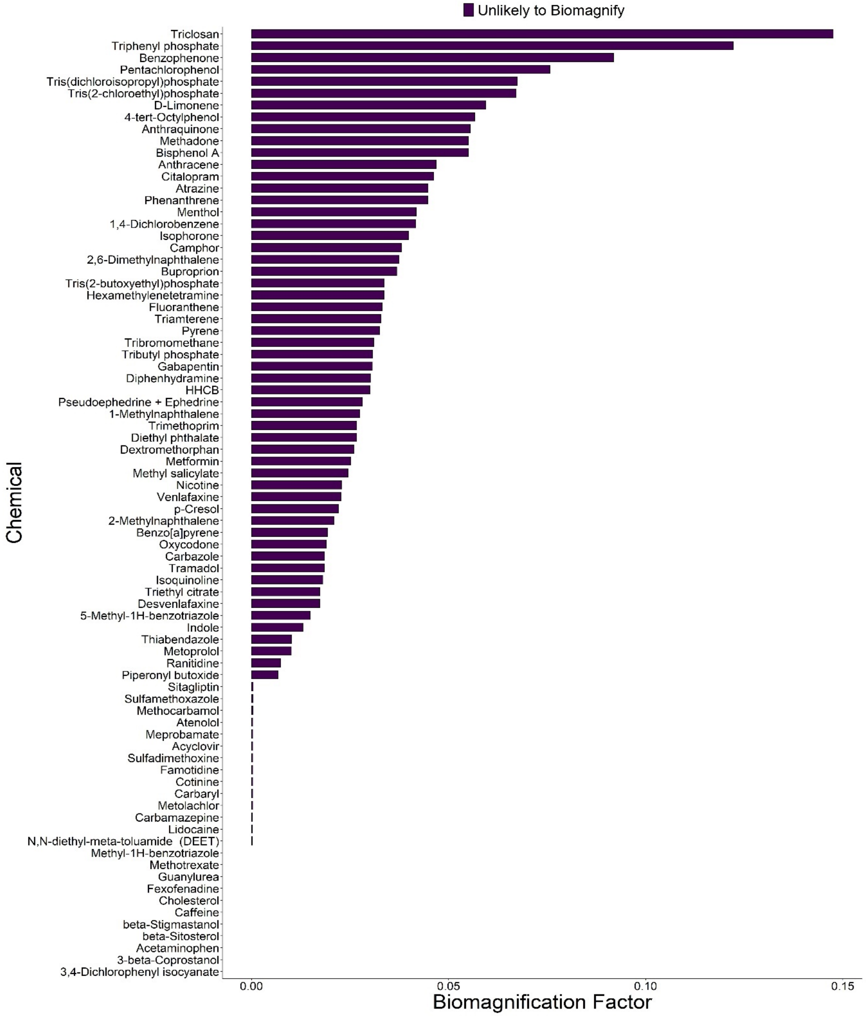
QSAR-estimated/experiment $t_{1/2}$
(ECHA; vPvB classification)

Bioaccumulation



QSAR-estimated/experimental BCF
(ECHA; vPvB classification)

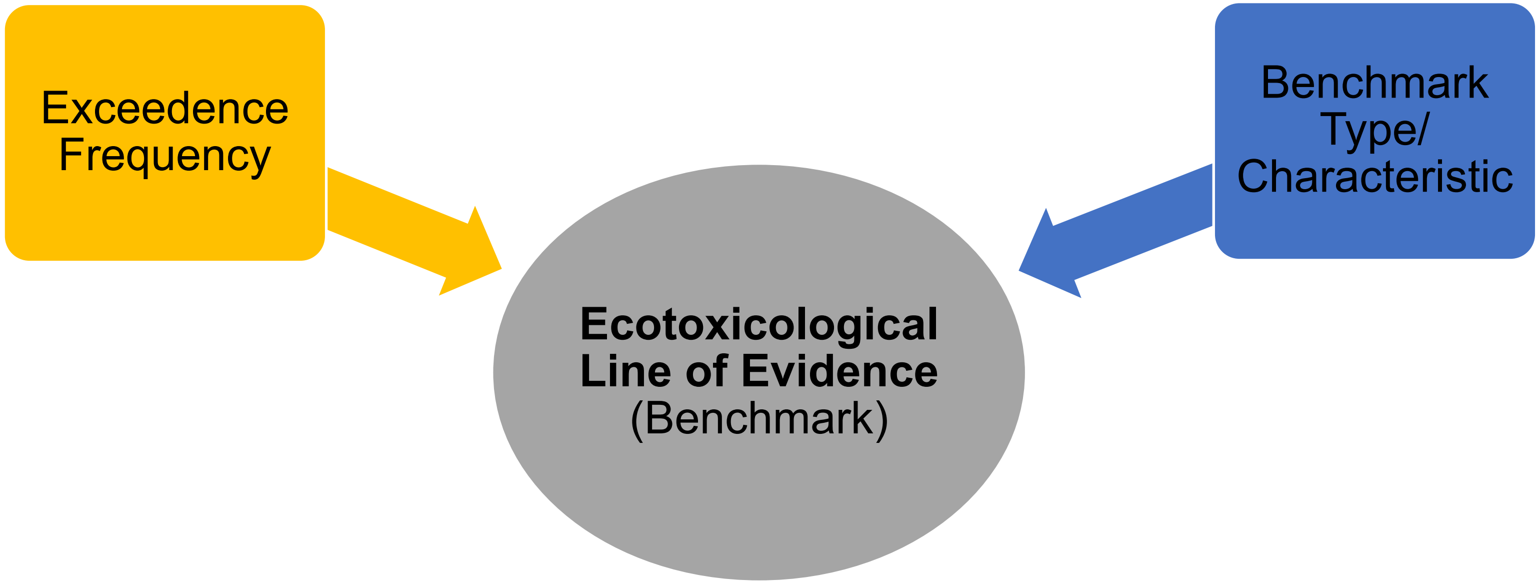
Biomagnification



QSAR-estimated/experimental BMF
(Gobas et al., 2009)

Ecotoxicological Benchmarks

- Each ecotoxicological benchmark was evaluated using a two-pronged approach:

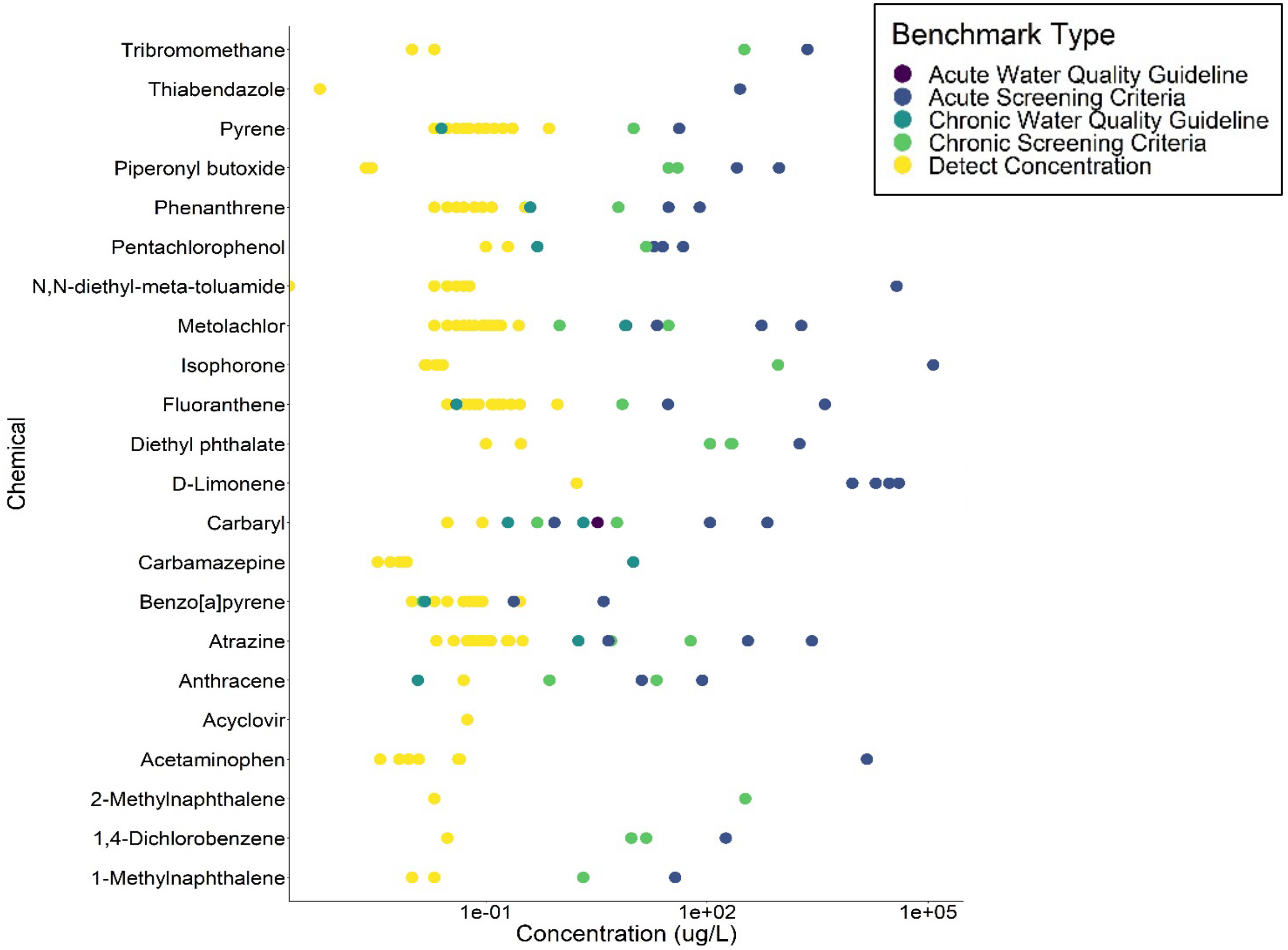


$$Final\ PS_{ecotox} = PS_{exceed\_freq}\ x\ \ Coefficient_{benchmark\_type}$$

Ecotoxicological Benchmarks

Water Quality Benchmarks

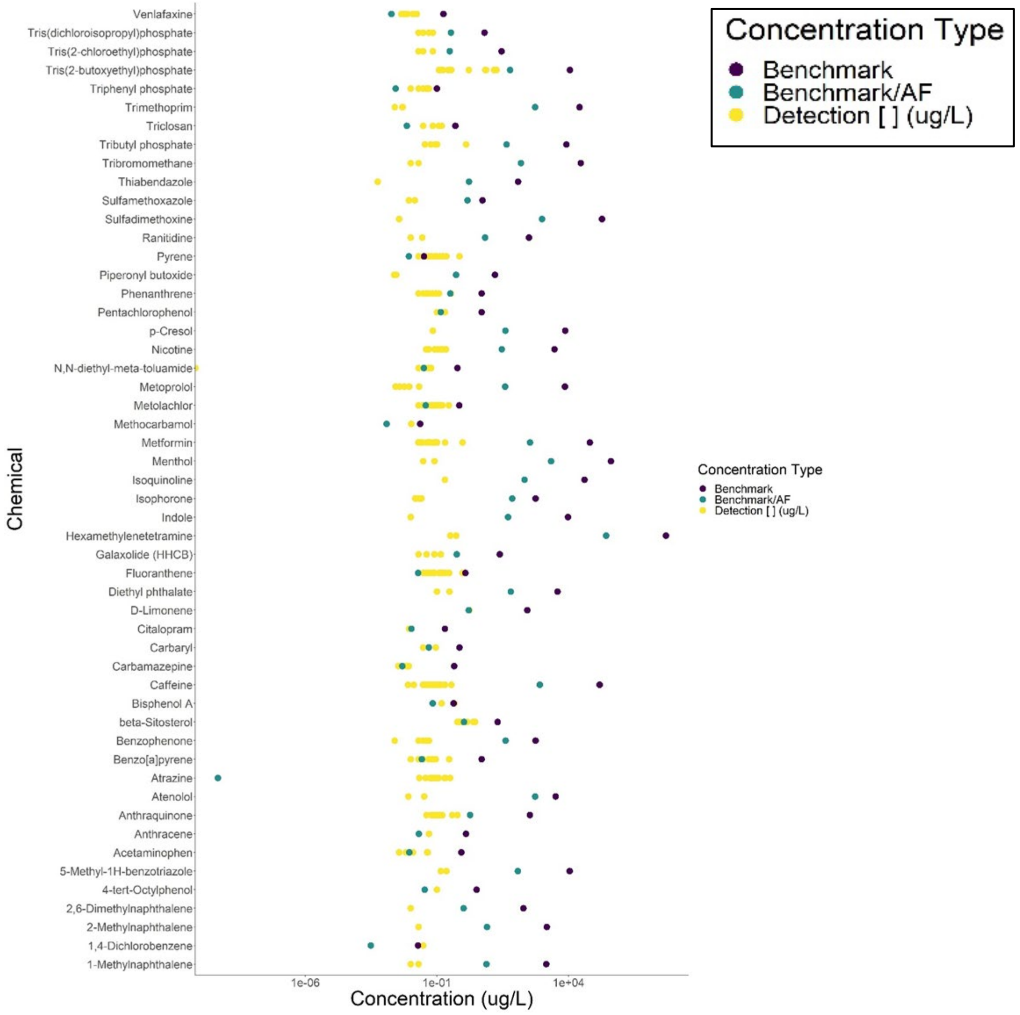
PS = 0 - 15



Canadian and US Water Quality Criteria + Screening Values.

ECOTOX Benchmarks

PS = 0 - 10



Application-factor adjusted and unadjusted *vivo* effect concentrations from the ECOTOX Knowledgebase.

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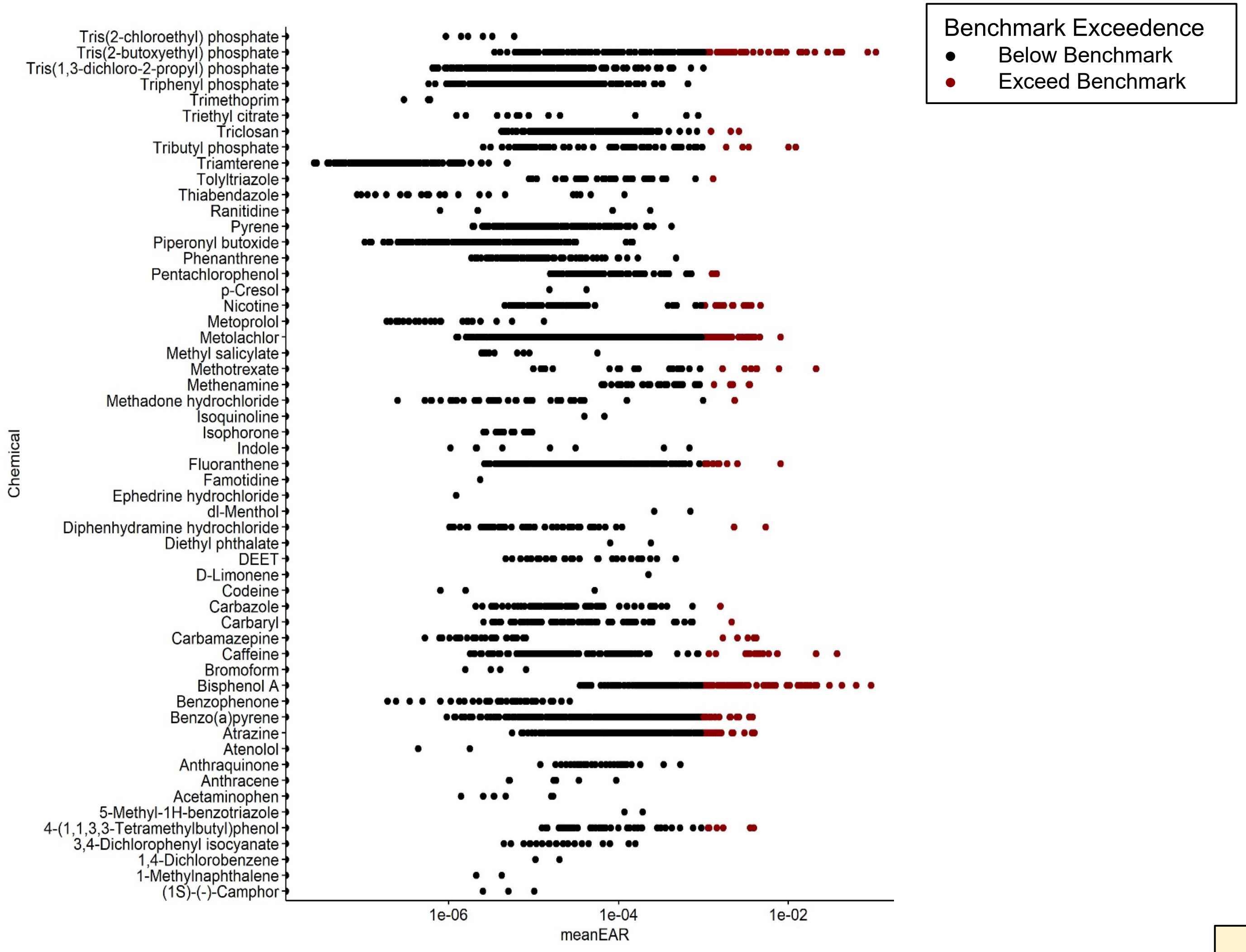
Ecotoxicological Benchmarks

ToxCast Benchmarks

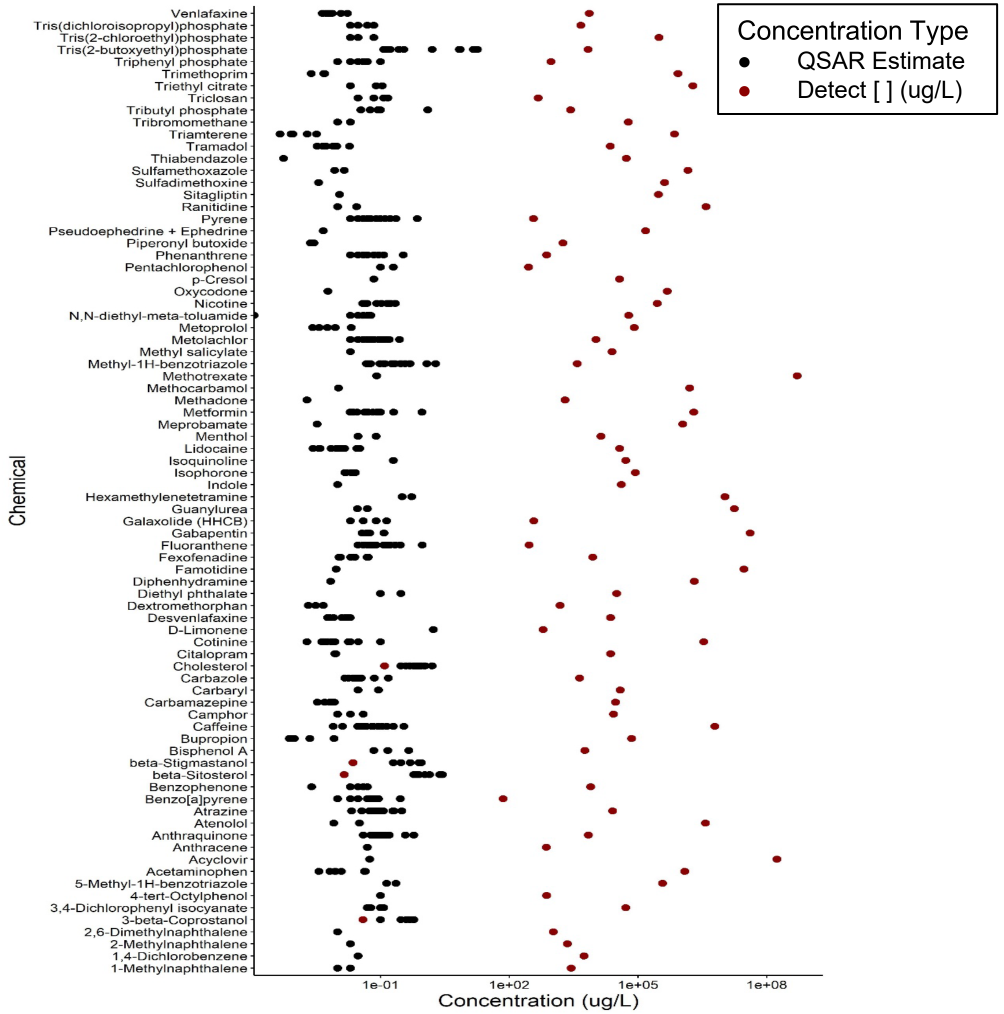
PS = 0 - 5



Minimum activity concentration at cut-off (ACC) derived from ToxCast database.

QSAR Benchmarks

PS = 0 - 5

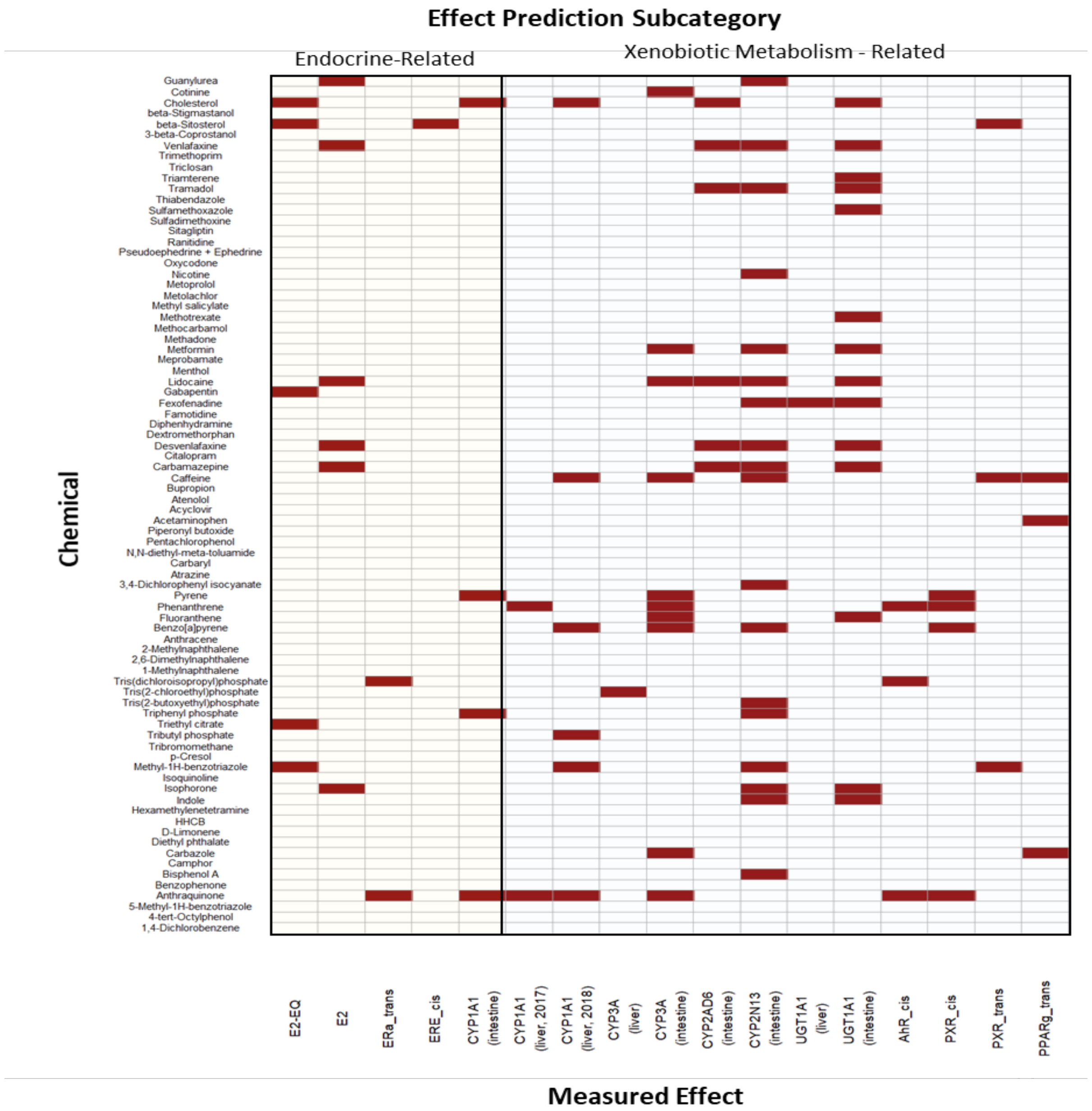


Unadjusted and application-factor adjusted consensus acute toxicity estimates derived from QSARs (TEST, ECOSAR, VEGA).

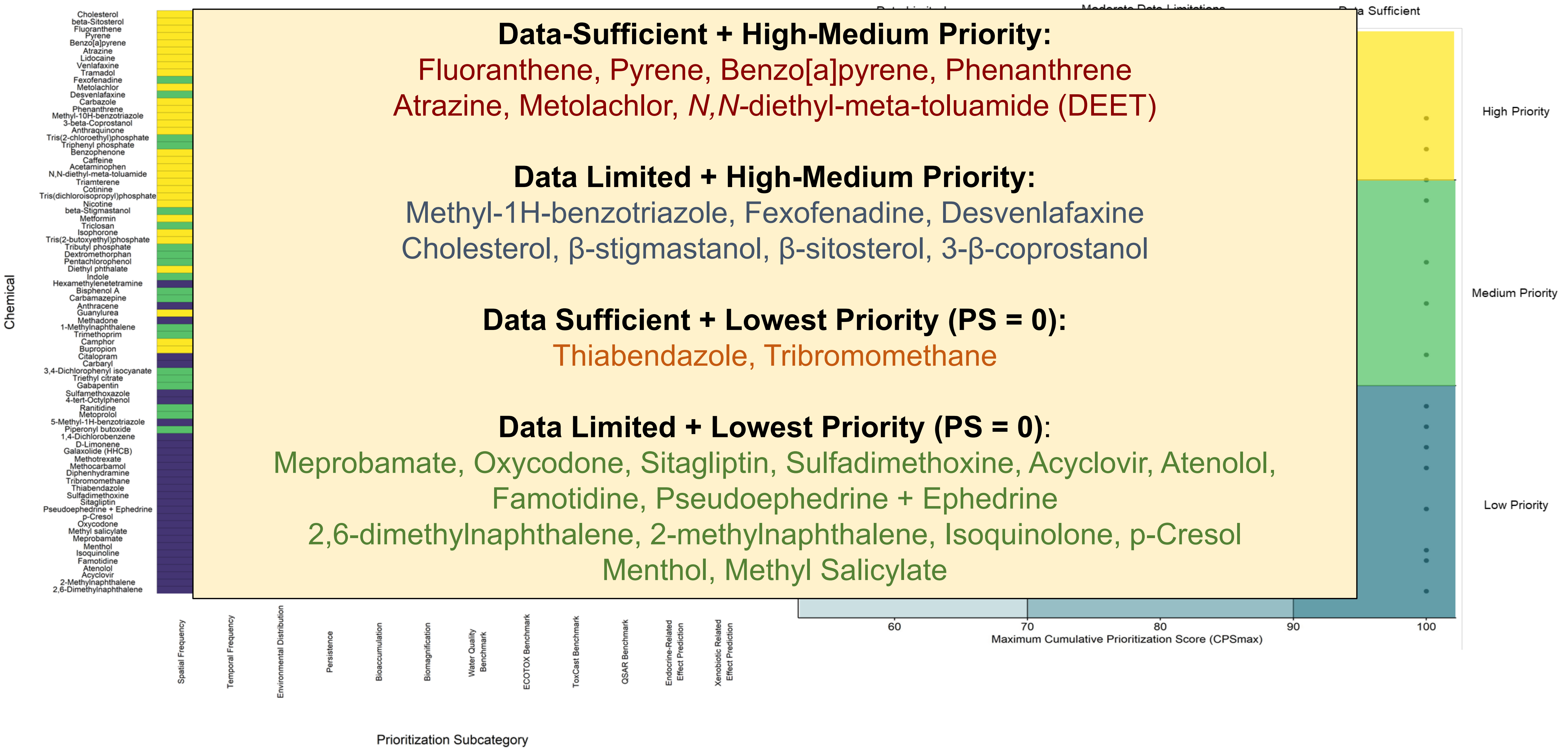
Effect Prediction

PS = 0 – 2.5

- Chemicals prioritized based on predictive relationships with endocrine- and xenobiotic metabolism-related effects.
- Random forest regression used to generate predictive models – 'important' chemical predictors identified for each effect.
- Weight-of-evidence used to identify priority compounds across effect prediction categories.



WoE Prioritization: Milwaukee Estuary



Data-Sufficient + High-Medium Priority:

Fluoranthene, Pyrene, Benzo[a]pyrene, Phenanthrene
Atrazine, Metolachlor, *N,N*-diethyl-meta-toluamide (DEET)

Data Limited + High-Medium Priority:

Methyl-1H-benzotriazole, Fexofenadine, Desvenlafaxine
Cholesterol, β-stigmastanol, β-sitosterol, 3-β-coprostanol

Data Sufficient + Lowest Priority (PS = 0):

Thiabendazole, Tribromomethane

Data Limited + Lowest Priority (PS = 0):

Meprobamate, Oxycodone, Sitagliptin, Sulfadimethoxine, Acyclovir, Atenolol,
Famotidine, Pseudoephedrine + Ephedrine
2,6-dimethylnaphthalene, 2-methylnaphthalene, Isoquinolone, p-Cresol
Menthol, Methyl Salicylate

Study Highlights and Key Findings

- Prioritized of 80 chemicals detected in the Milwaukee Estuary AOC based on *detection characteristics*, *environmental fate*, *ecotoxicological potential, effect prediction, & data availability.*
  - **7 high-priority, data sufficient compounds** = candidates for further effects-based monitoring efforts.
  - **7 high – medium-priority, data limited compounds** = candidates for further ecotoxicological characterization.
  - **2 low-priority, data sufficient compounds** = definitively low priority compounds.
  - **14 low-priority, data limited compounds** = potential low priority compounds.

Developed an alternative prioritization framework that can be employed or adapted to transparently prioritize contaminants within freshwater watersheds. *Maloney et al. 2021, in prep.*

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Thank you for your attention!

Questions, Comments?

Contact: malon625@d.umn.edu or leave a comment below!