Application of RISK21 Framework in regulatory based decision making:
From business decisions to prioritization to risk assessment

# High-throughput risk-based prioritization for ecological risk assessment

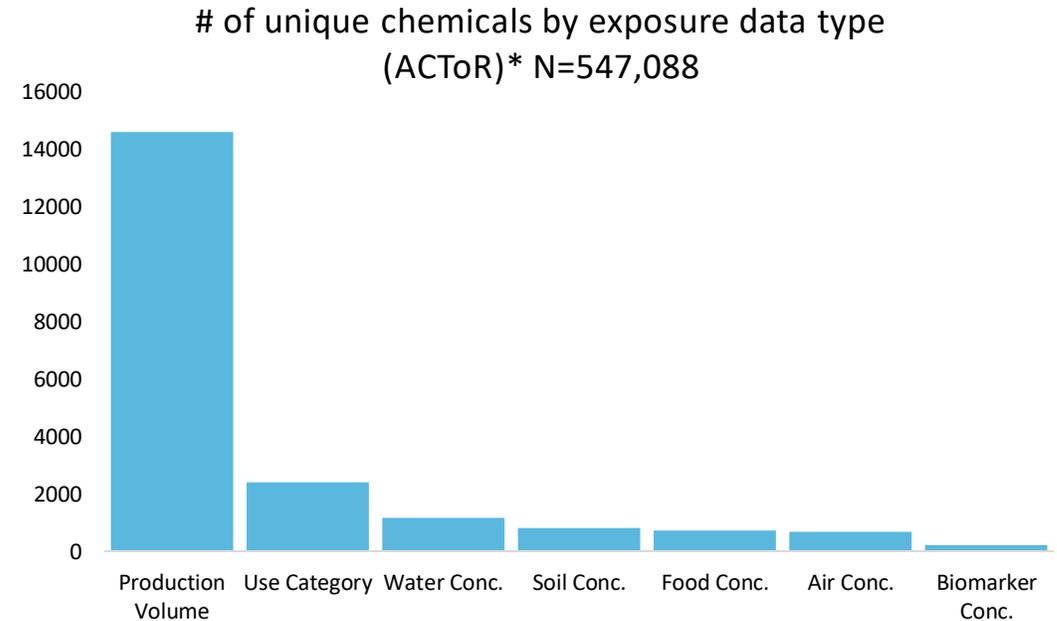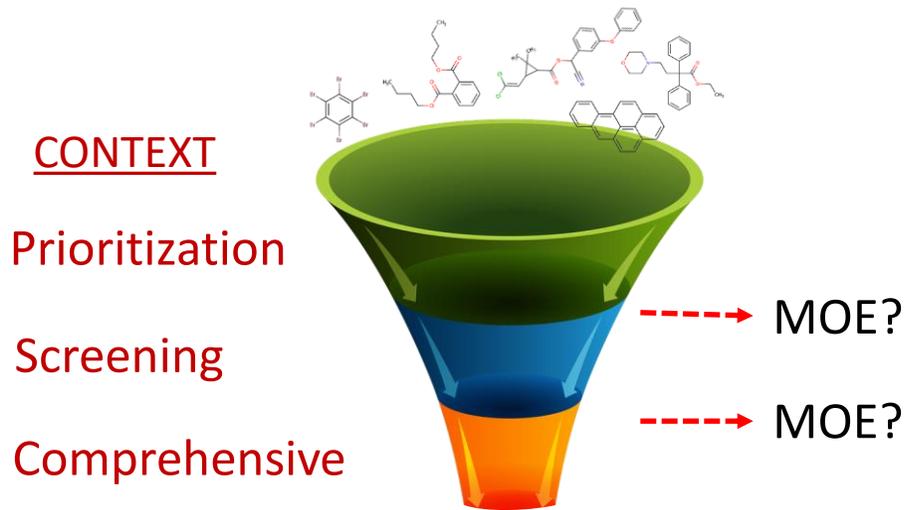Jon Arnot

Webinar – May 19, 2020

# Presentation overview

- Background: Ecological risk-based prioritization methods

- Risk Assessment, IDentification And Ranking (RAIDAR) model

- Screen 12,000 organic chemicals for ecological risks

- Examine some of the results in the RISK21 framework (matrix)

- Compare <u>holistic risk-based</u> prioritization vs. <u>PBT classifications</u> (current TSCA?)

- Summary
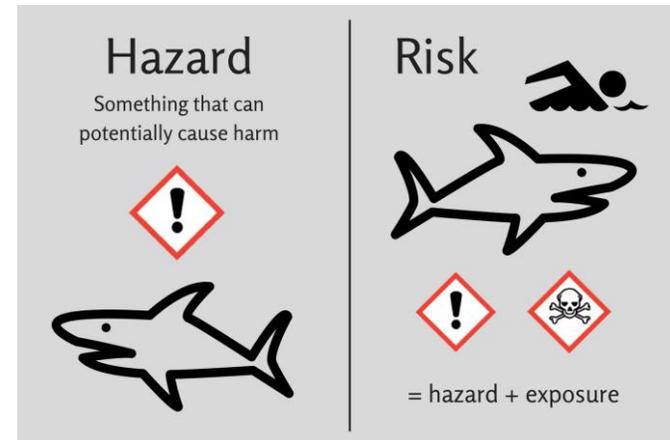
# Global regulatory situation

- Many diverse chemicals and use contexts require evaluation

- Limited information → uncertainty (i.e., **exposure**)

- Need to develop, evaluate and apply **databases** and **models** for different contexts, i.e., "**fit-for-purpose**"

CONTEXT

Prioritization

Screening

Comprehensive

----→ MOE?

----→ MOE?

# of unique chemicals by exposure data type
(ACToR)* N=547,088

*USEPA's Aggregated Computational Toxicology Online Resource*

*Egeghy et al, 2012*

# Tiered Approach to Risk-Based Decision-Making, e.g., RISK21

Which organic chemicals are likely to pose the greatest risks to ecological receptors?

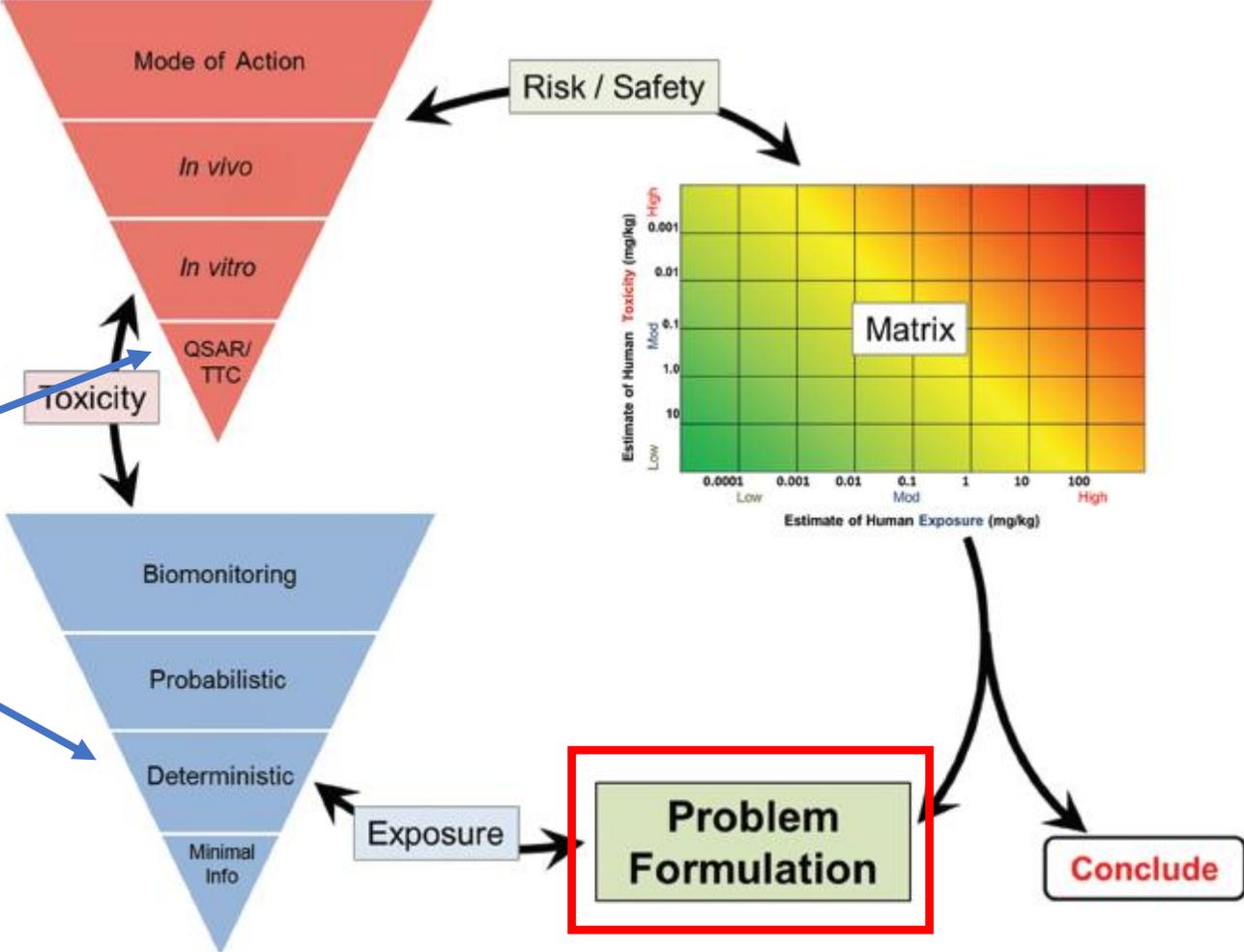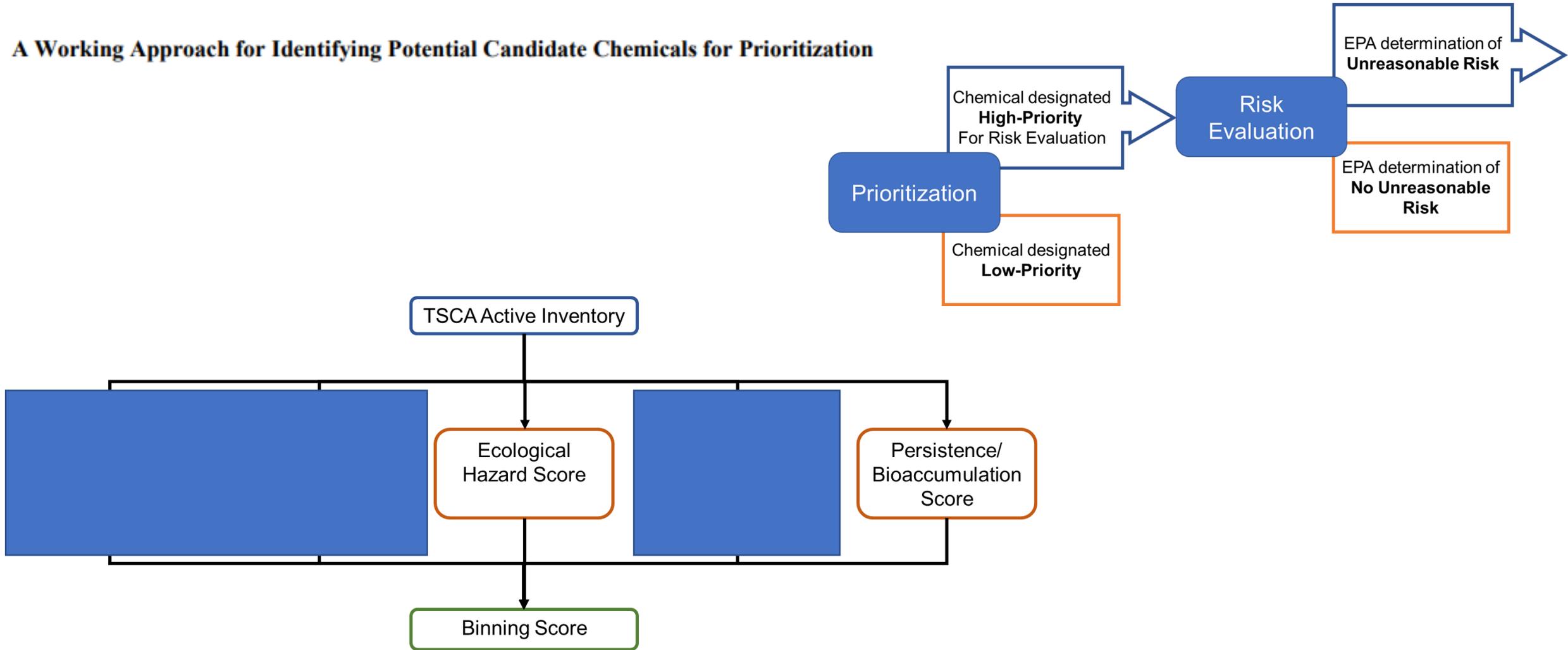**Tier 1:** Screen and prioritize a large number of organic chemicals using currently available data



Figure 2. General conceptual framework of the RISK21 approach.

Embry et al. Crit. Rev. Tox. 2014

**EPA**

United States
Environmental Protection Agency

September 27, 2018
Office of Chemical Safety and
Pollution Prevention

## A Working Approach for Identifying Potential Candidate Chemicals for Prioritization

Chemical designated **High-Priority** For Risk Evaluation

Risk Evaluation

EPA determination of **Unreasonable Risk**

EPA determination of **No Unreasonable Risk**

Prioritization

Chemical designated **Low-Priority**

TSCA Active Inventory

Ecological Hazard Score

Persistence/ Bioaccumulation Score

Binning Score

# PBT Approach: multi-category classification

| Category | TSCA (maybe?) | |
| --- | --- | --- |
| | Moderate (Action Level) | High (Action Level) |
| **Persistence** | Chemical half-life:<br>> 60 d in water or<br>> 60 d in soil or<br>> 60 d in sediment | Chemical half-life:<br>> 180 d in water or<br>> 180 d in soil or<br>> 180 d in sediment |
| **Bioaccumulation** | BCF or BAF in fish > 1000 L/kg-ww | BCF or BAF in fish > 5000 L/kg-ww |
| **Toxicity** | Acute Aquatic Toxicity - L(E)C50<br>> 10 – 100 mg/L<br>Chronic Aquatic Toxicity - L(E)C50<br>> 1 – 10 mg/L | Acute Aquatic Toxicity - L(E)C50<br>≤ 10 mg/L<br>Chronic Aquatic Toxicity - L(E)C50<br>≤ 1 mg/L |

EPA TSCA Work Plan Chemicals: Methods Document February 2012

# PBT Approach: multi-category classification

| Category | TSCA (maybe?) | |
| :---: | :---: | :---: |
| | **Moderate (Action Level)** | **High (Action Level)** |
| **Persistence** | Chemical half-life:<br>> 60 d in water or<br>> 60 d in soil or<br>> 60 d in sediment | **Chemical half-life:**<br>**> 180 d in water or**<br>**> 180 d in soil or**<br>**> 180 d in sediment**    **> 2 d in air** |
| **Bioaccumulation** | BCF or BAF in fish > 1000 L/kg-ww | **BCF or BAF in fish > 5000 L/kg-ww** |
| **Toxicity** | Acute Aquatic Toxicity - L(E)C50<br>> 10 − 100 mg/L<br>Chronic Aquatic Toxicity - L(E)C50<br>> 1 − 10 mg/L | Acute Aquatic Toxicity - L(E)C50<br>≤ 10 mg/L<br>**Chronic Aquatic Toxicity - L(E)C50**<br>**≤ 1 mg/L** |

# RAIDAR model concepts

Combines mass balance **fate** and **bioaccumulation** models to link chemical emissions to **<span style="color:red">exposure</span>** (and **hazard** for **<span style="color:red">risk</span>**)
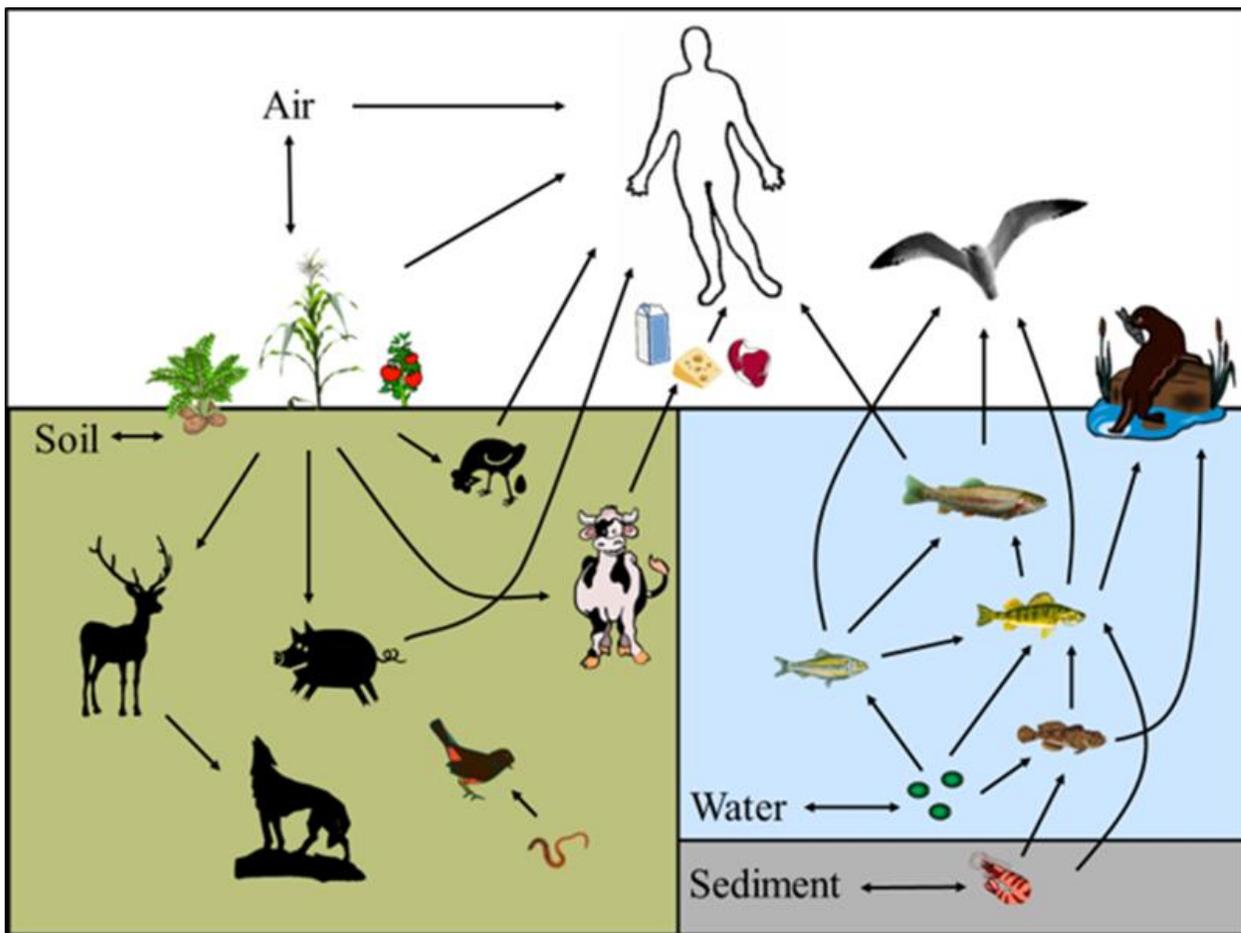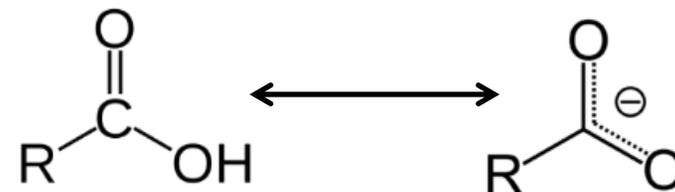


Evaluative, regional scale, steady-state

Representative ecological receptors

Far-field human exposure

Environmental and biological concentrations
Persistence (e.g., $P_{OV}$), LRTP
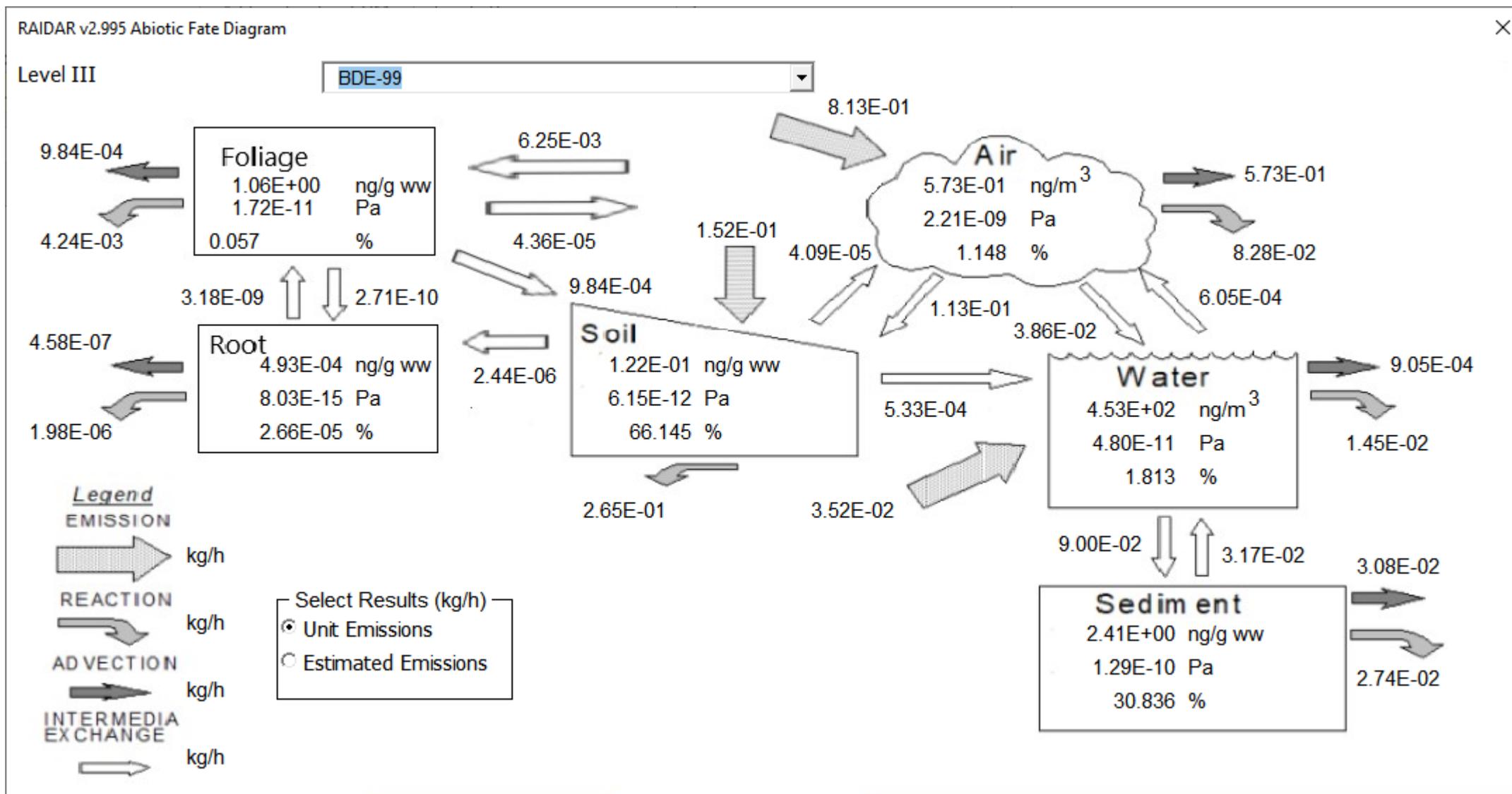Bioaccumulation metrics (e.g., BCF, BAF, BMF)



Ver.1.0: Arnot et al. *ES&T* 2006     Ver.2.0: Arnot and Mackay *ES&T* 2008
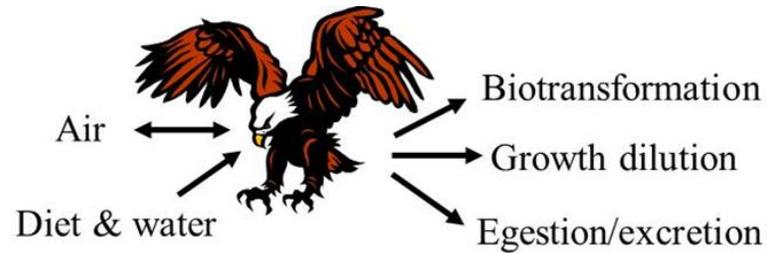
Ver.3.0: Arnot et al., in prep.
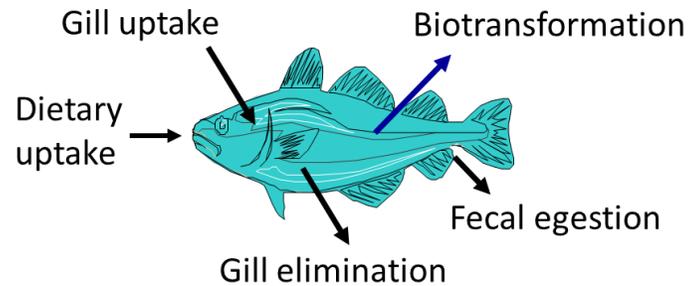
# Quantify chemical fate using mass balance models

# Quantify chemical exposure using mass balance models

**Air-respiring organisms ($K_{OW}$ + $K_{OA}$)**



**Water-ventilating organisms ($K_{OW}$)**





RAIDAR v2.995 Foodweb Results

**Air**

| Terrestrial Carnivore | | Human | | Avian omnivore-scavenger | |
| --- | --- | --- | --- | --- | --- |
| 7.14E-01 ug/kg ww | | 8.69E+01 ug/kg ww | | 1.87E+03 ug/kg ww | |

| | | | | |
| --- | --- | --- | --- | --- |
| | Poultry1-Broiler | 2.11E+00 ug/kg ww | Poultry2-Layer | 1.07E+00 ug/kg ww |
| | Pig | 2.75E+00 ug/kg ww | Egg | 1.07E+00 ug/kg ww |
| | Cow1-Beef | 6.82E-01 ug/kg ww | Cow2-Dairy | 5.82E-01 ug/kg ww |

Terrestrial Herbivore
3.61E-01 ug/kg ww

| Dairy Calf | 3.08E-01 ug/kg ww | |
| --- | --- | --- |
| Bulk Dairy | 1.25E-01 ug/kg ww | Aquatic Mammal |
| Milk | 6.63E-02 ug/kg ww | 1.83E+03 ug/kg ww |

Avian omnivore-small
4.64E+00 ug/kg ww

Foliage     1.06E+00 ug/kg ww

**Soil**

| Root | 4.93E-04 ug/kg ww |
| --- | --- |
| Soil Invertebrates | 7.22E-01 ug/kg ww |

**Freshwater**

| Planktivorous Fish | 1.19E+01 ug/kg ww |
| --- | --- |
| Benthivorous Fish | 2.50E+02 ug/kg ww |
| Omnivorous Fish | 3.17E+02 ug/kg ww |
| Piscivorous Fish | 5.90E+02 ug/kg ww |
| Aquatic Invertebrates: | 3.68E+01 ug/kg ww |
| Zooplankton | 5.39E+00 ug/kg ww |
| Phytoplankton | 2.37E+00 ug/kg ww |

BDE-99

**Options**

**Emissions**
- ● Unit Emission (1 kg/h)
- ○ Estimated Emission (kg/h)

**View Results**
- ● Concentration (ug/kg ww)
- ○ Fugacity (Pa)

**Sediment**

| Benthic Invertebrates | 1.86E+02 ug/kg ww |
| --- | --- |

# RAIDAR input requirements: "PBT" information

| | |
|---|---|
| Molar mass | |
| Octanol-water partition coefficient ($K_{OW}$) | Chemical properties |
| Air-water partition coefficient ($K_{AW}$) | |
| Dissociation constant (Ka) | |
| Reaction rate (or half-life) in air | |
| Reaction rate (or half-life) in water, soil and sediment | Degradation properties |
| Reaction rate (or half-life) in biota (fish, mammals) | |
| Chemical emission rate | |
| Mode-of-entry (application/use) | Chemical usage: How much? How? |
| Toxicity data for risk calculations | Hazard data, e.g., LC50, IEC50, TTC |

# Eco-risk high-throughput screening & prioritization

12,000 organic chemicals

Production volume bins (geomean) for emissions estimate
Databases and QSAR predictions for other input parameters
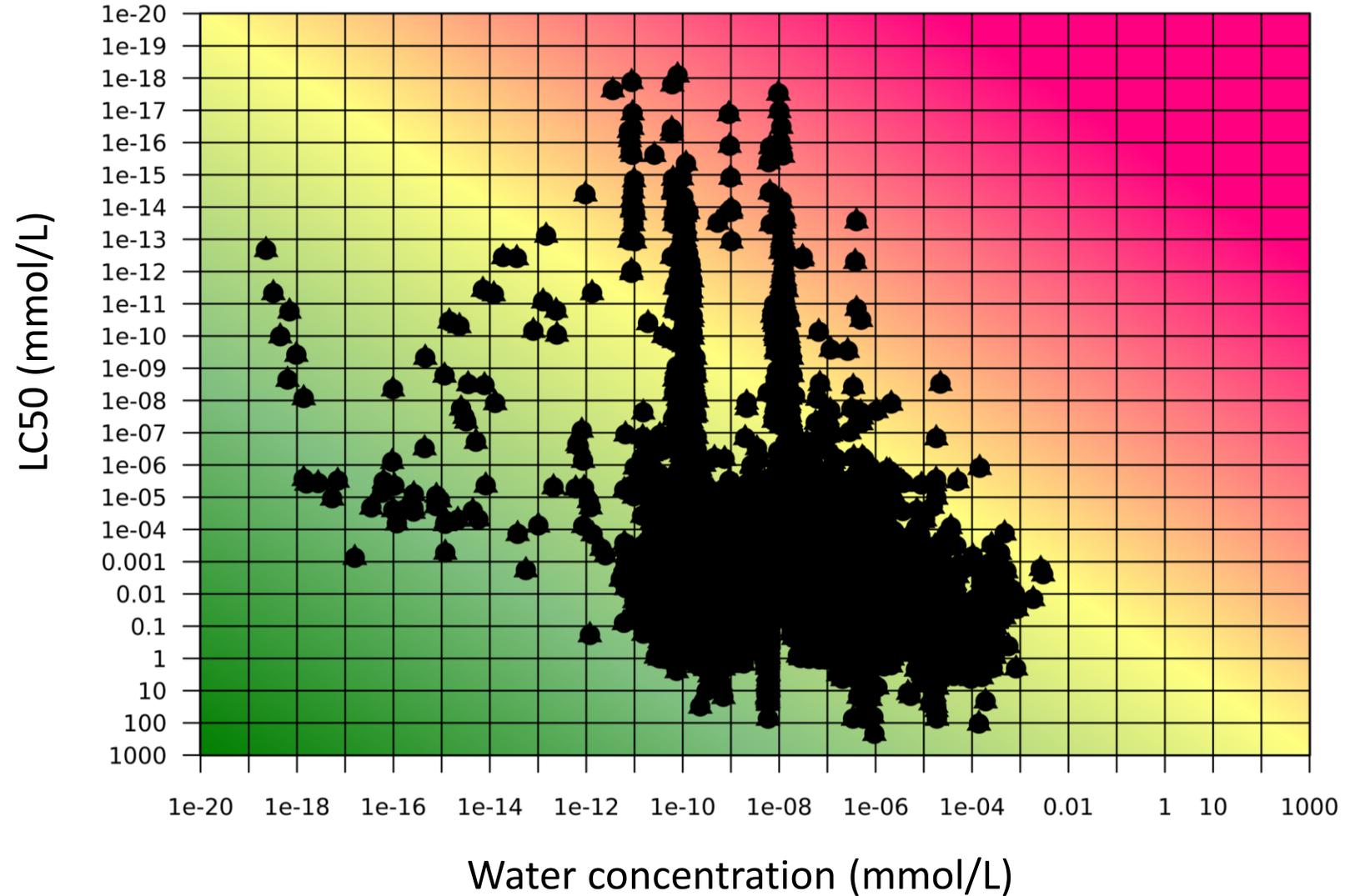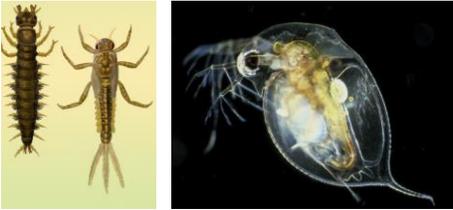Same basic information used in PBT assessments

5. Compare RAFs (risk-based) and PBT classification (hazard-based) results for prioritization
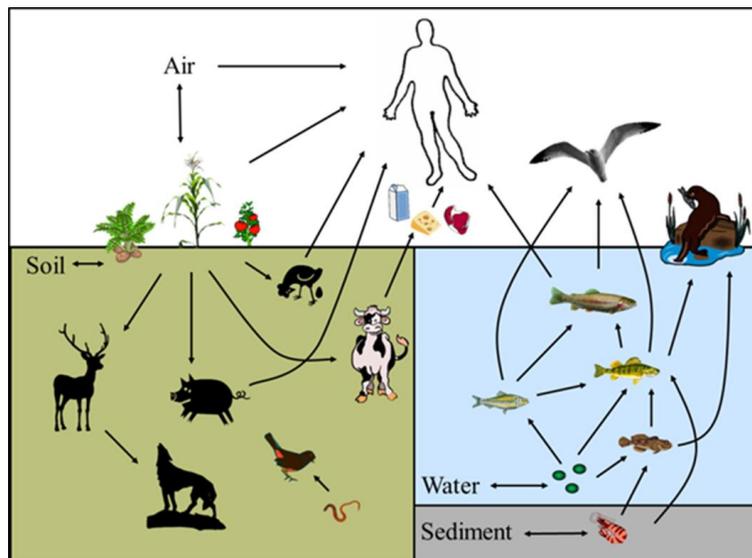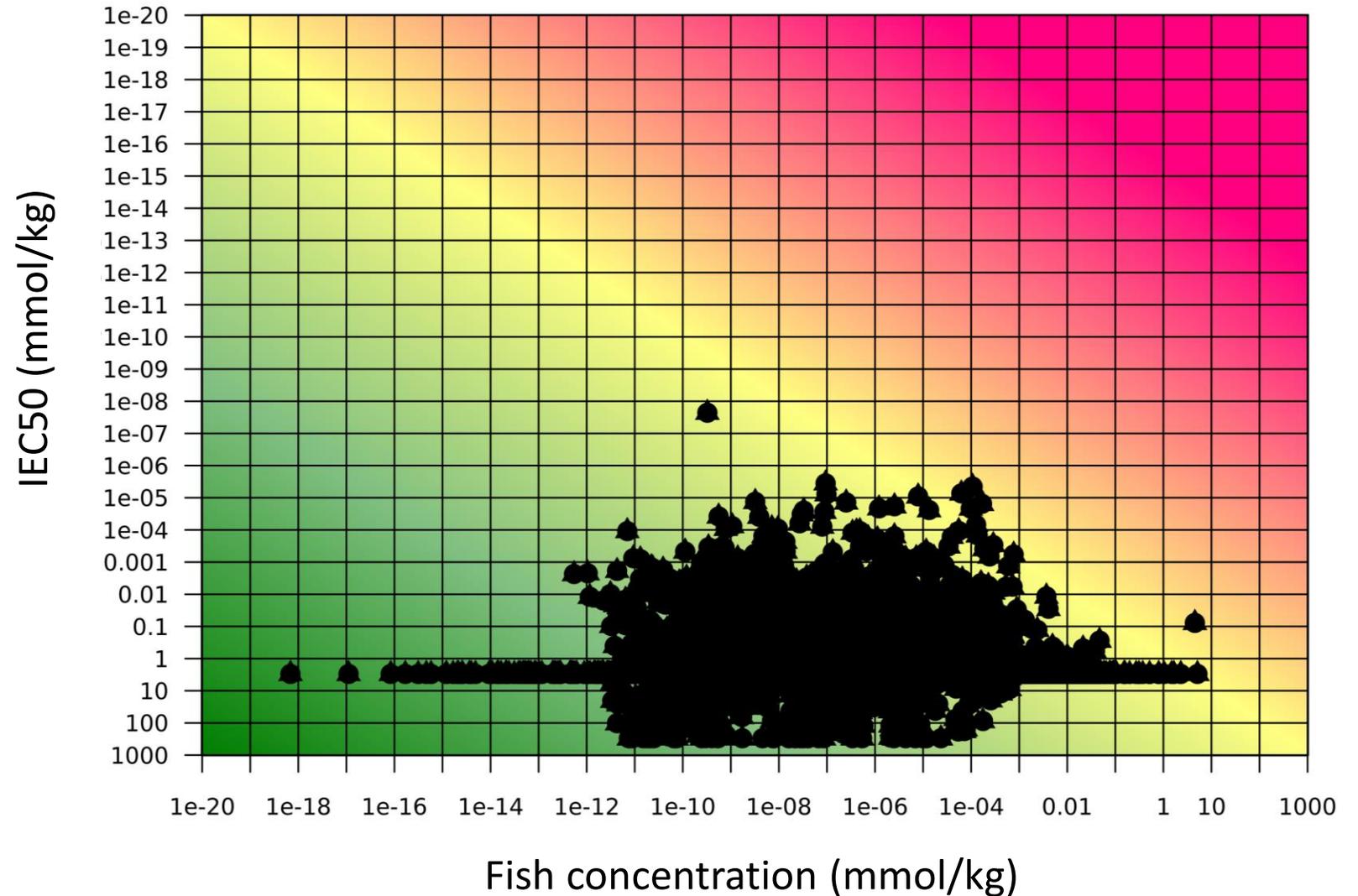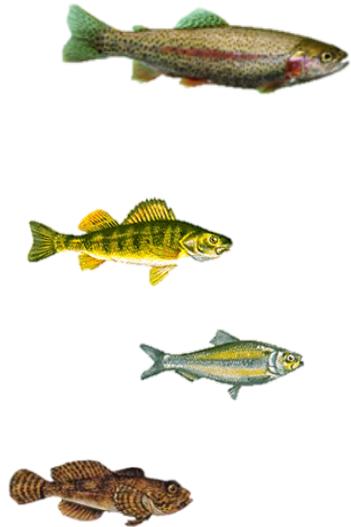


**RAIDAR output**

1. Environmental concentrations
2. Biological concentrations
3. Biota intake rates
4. Risk Assessment Factors (**RAFs**)
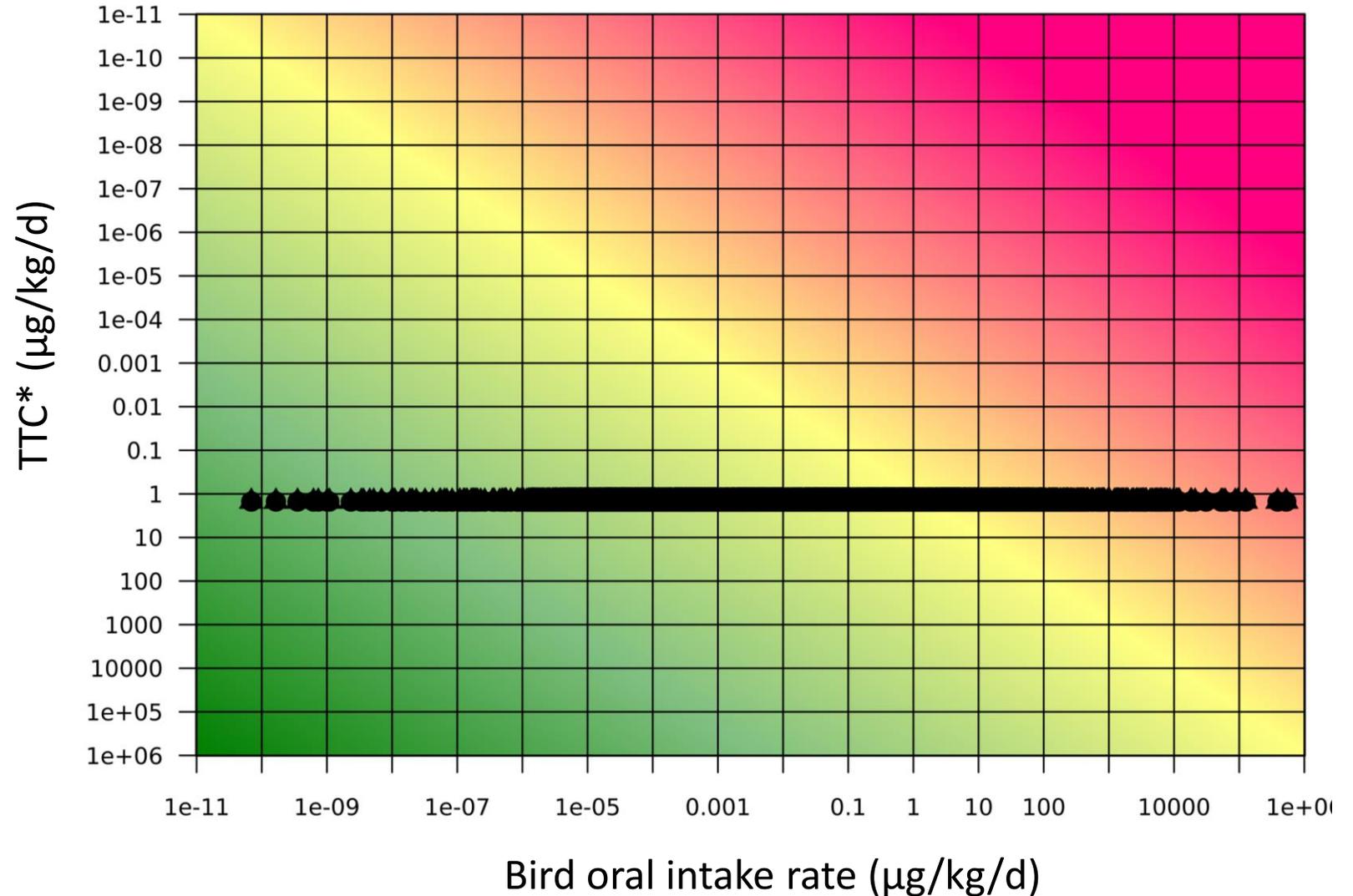
Arnot et al., in prep

# 1. Predicted water concentrations vs. LC50
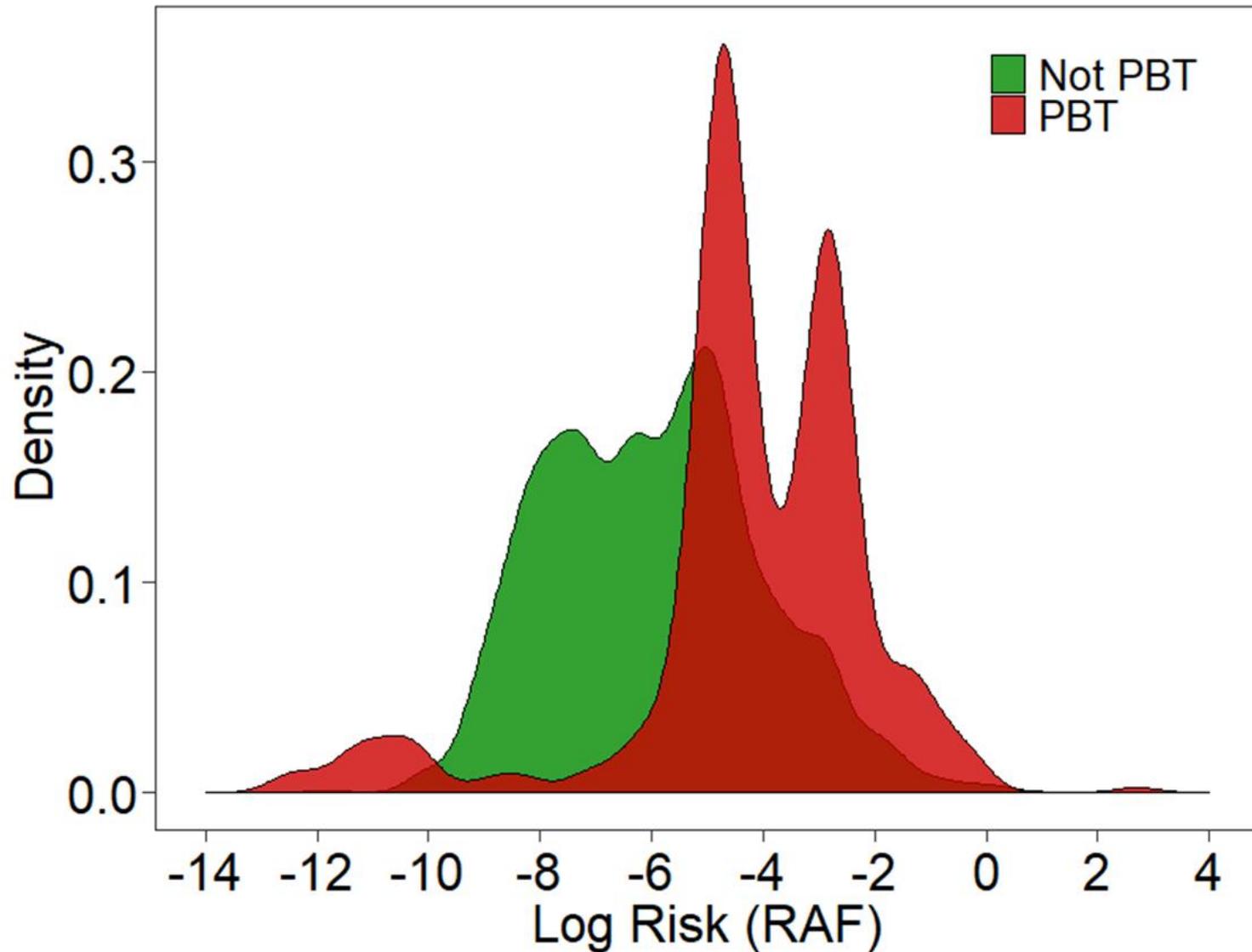
# 2. Predicted fish concentrations vs. IEC50

# 3. Predicted intake rates (e.g., bird) vs. TTC



*Cramer Class III
5th-%ile NOEL/100

# 4 & 5. Comparison of results from the two methods….



1. Many "PBT" chemicals are of relatively low risk

2. Many "non-PBT" chemicals have relatively equal or greater risk than "PBTs"

Used aquatic toxicity data <u>only</u>

Arnot et al., in prep

# Summary

- RISK21 tiered approach can be used for ecological assessments

- Models and data exist to conduct holistic exposure and risk-based screening and prioritization for more comprehensive ecological health assessment

- Many chemicals regulated as "PBT" are not likely "risks" – **FALSE POSITIVES**

- Many chemicals "not PBT" may pose risks – **FALSE NEGATIVES**

- **P & B Criteria ≠ Exposure; PBT Criteria ≠ Risk**

- Uncertainty analysis can be included in RAIDAR; not addressed in "PBT" approach

- On-going work…
  - More RAIDAR evaluations with monitoring data to foster confidence in exposure modelling
  - Revisions to substance flow model (CiP-CAFE) to address uncertainty in chemical emissions

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**Questions?**

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