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Application of equilibrium partitioning-based model framework for evaluating soil (and sediment) hazards of lipophilic nonpolar organic substances.

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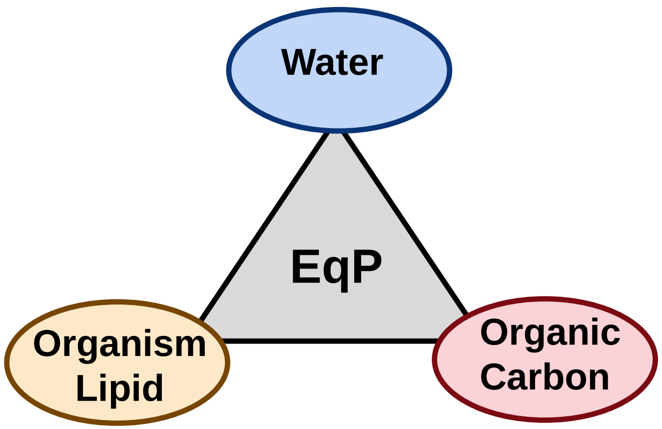
Case Study 3
Topical Scientific Workshop on Soil Risk Assessment
Date and Time of Talk: Wednesday, October 7, 2015
Location: Helsinki

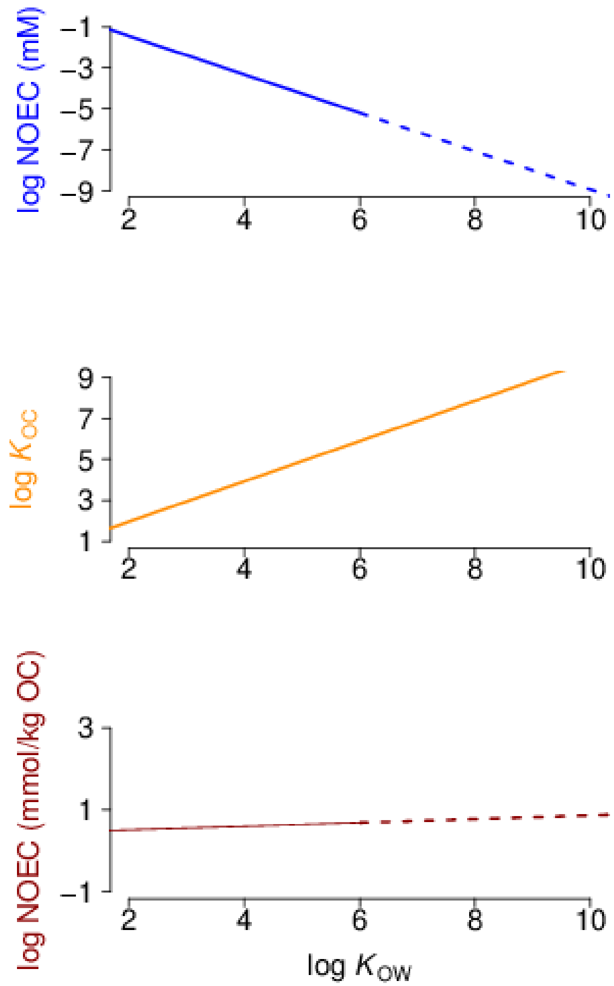
outline

- Objective: Extension of target lipid model (TLM) for soil (and sediment) hazard and risk assessment using Equilibrium Partitioning (EqP)
  - TLM-EqP, *Env. Toxicol. Chem.* (2014) 33:2679-2687
- Establish technical basis for extrapolation of TLM-EqP
- Application of framework to inform registration strategy for very hydrophobic substances
  - Synthetic engine oil (C20-22 alkanes, logK_{OW} 10-12)
  - Synthetic ester lubricant (C35 nonionic ester blend, logK_{OW} ~12)

Conceptual model

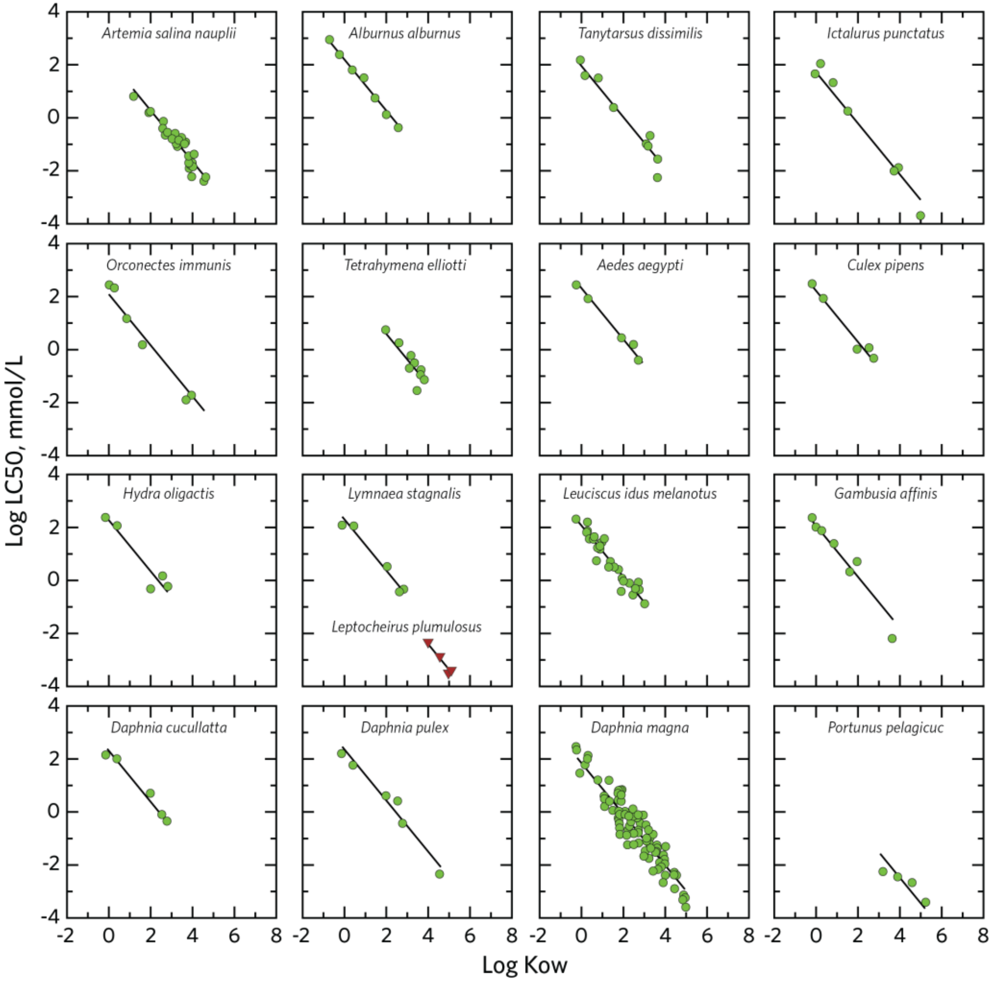
- Equilibrium Partitioning – expecting consistency between results from different media, routes of exposure (diet + porewater)
  - Application of logK_{OC} provides a means for this transformation.





Development of QSAR for Aquatic Exposures

- Target Lipid Model
  - Initial calibration based on aquatic exposures
    - Data availability
  - Critical Target Lipid body burden model (CTLBB)
  - >80 species in total
    - McGrath and Di Toro 2009; HDR 2015



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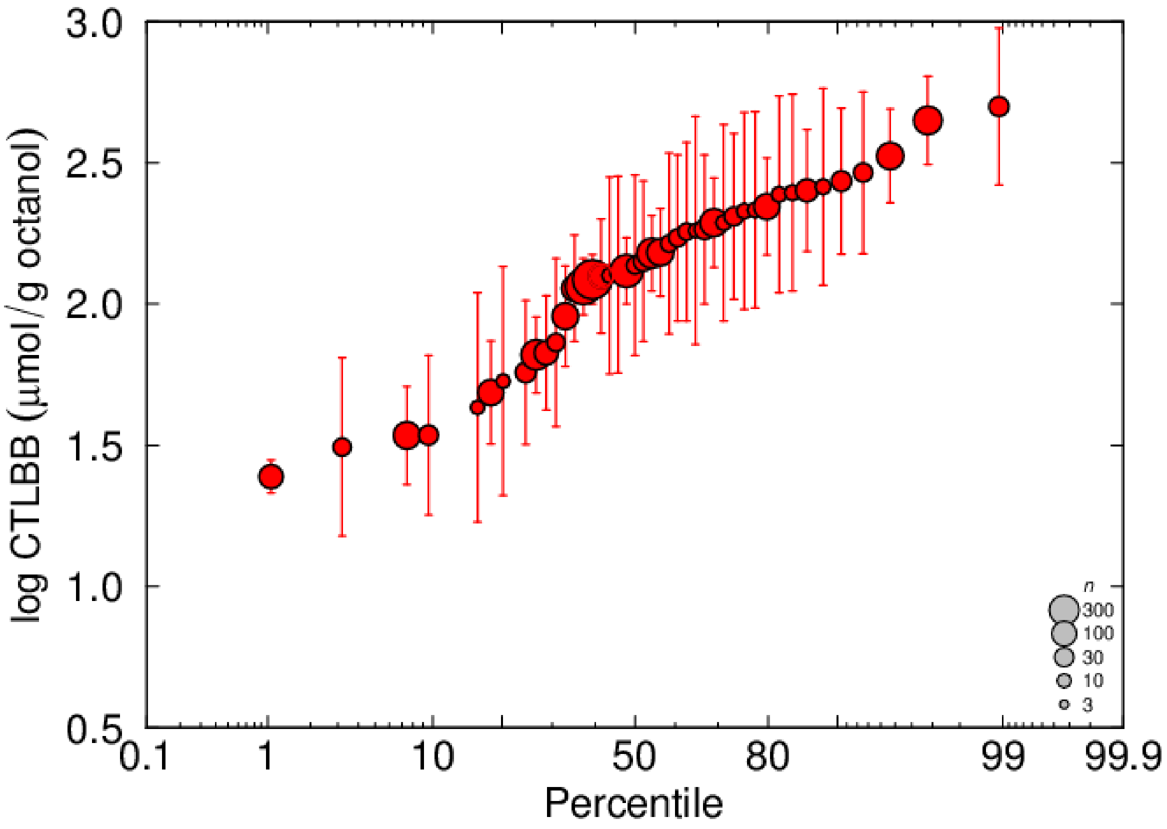
Sensitivity Distribution for Aquatic Exposures

- TLM-derived CTLBBs establish range of species sensitivity



Development of PNECs using TLM

- HC_5 extrapolation used to estimate PNECs
  - Statistics (mean and variance) of acute and chronic toxicity based
  - TLM-SSDs used to derive HC_5
  - Elements of HC5:

    K_{OW}, CTLBB, ACR, covariance

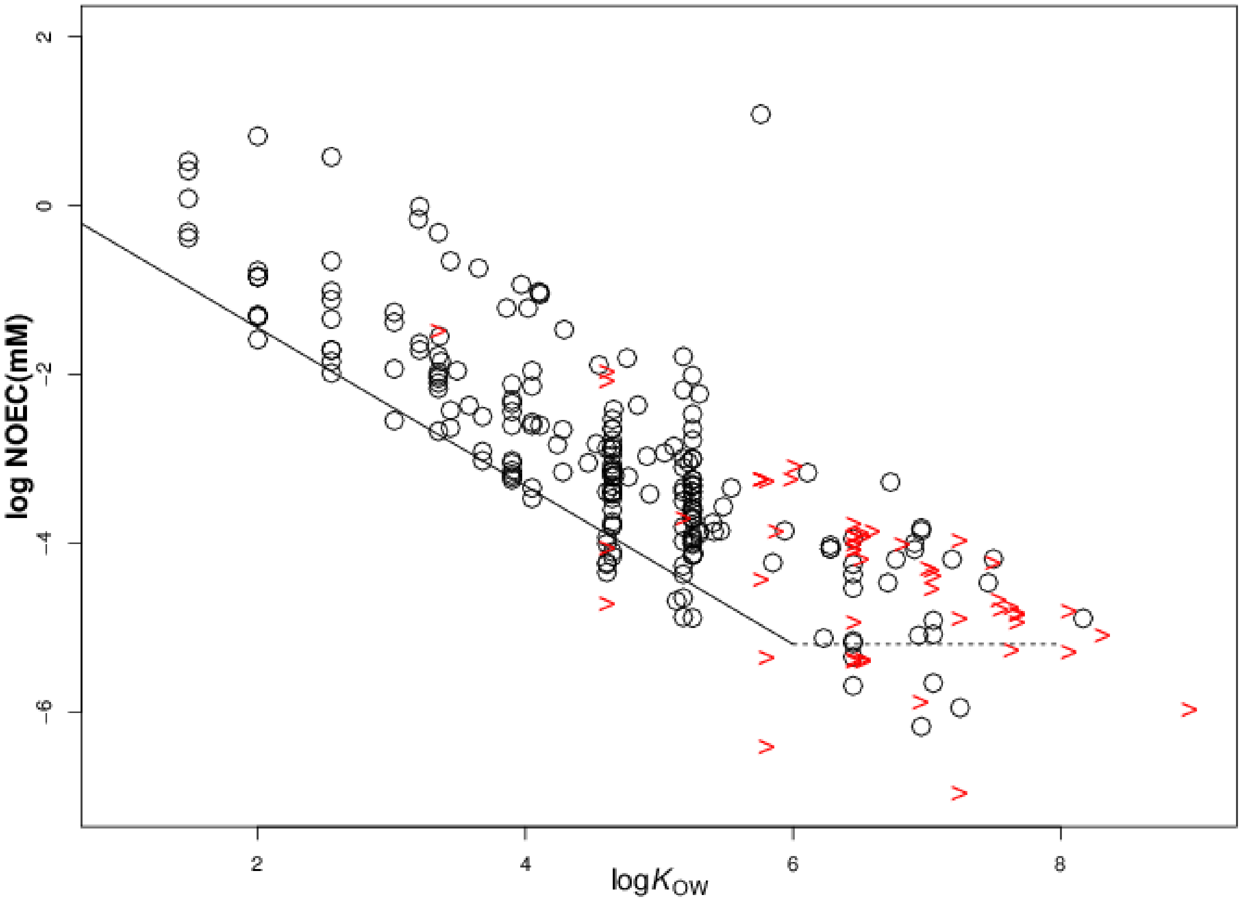
$$Log\ (HC_5) = E(m)\ log\ (K_{ow}) + E\{log(C^*_L)\} - E\{log\ (ACR)\}$$

$$-k_Z \sqrt{V\{m\}log(K_{OW})^2 + V\{log(ACR)\} + V\{log\ C^*_L\} + 2log(K_{ow})COV(m, logC^*_L)}$$

- Domain:
  - nonpolar organics up to logK_{OW} 6.0,
    - above this point toxicity is variable and uncertain

Validation of HC5

- Growing database of high quality chronic data
  - 35 species, 8 taxonomic classes, 170 individual entries
  - Multiple tests on substances with logK_{OW} > 6 are non-toxic at saturation (>)
    - Characterizes region of limited bioavailability for nonpolar organics



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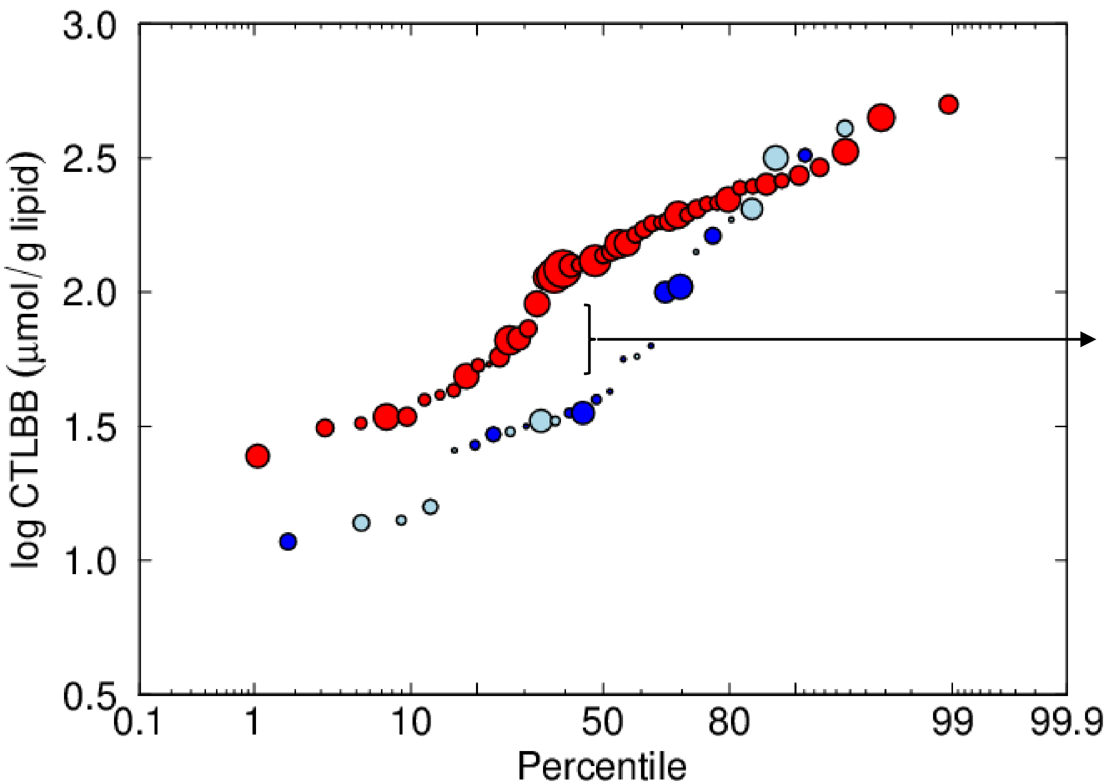
Comparing aquatic TLM to soil TLM

- Analogous TLM validation exercise conducted
  - Acute and chronic toxicity data (Klimisch score 1, 2) for nonpolar organics
  - Soil (and Sediment) data compiled (26 species: plant, annelids, insects, etc)
    - Assumed to include dietary exposure
  - Range of sensitivity is similar between compartments



Experimental artifact due to longer exposures in soil (i.e. 2-4d vs 14-28d)

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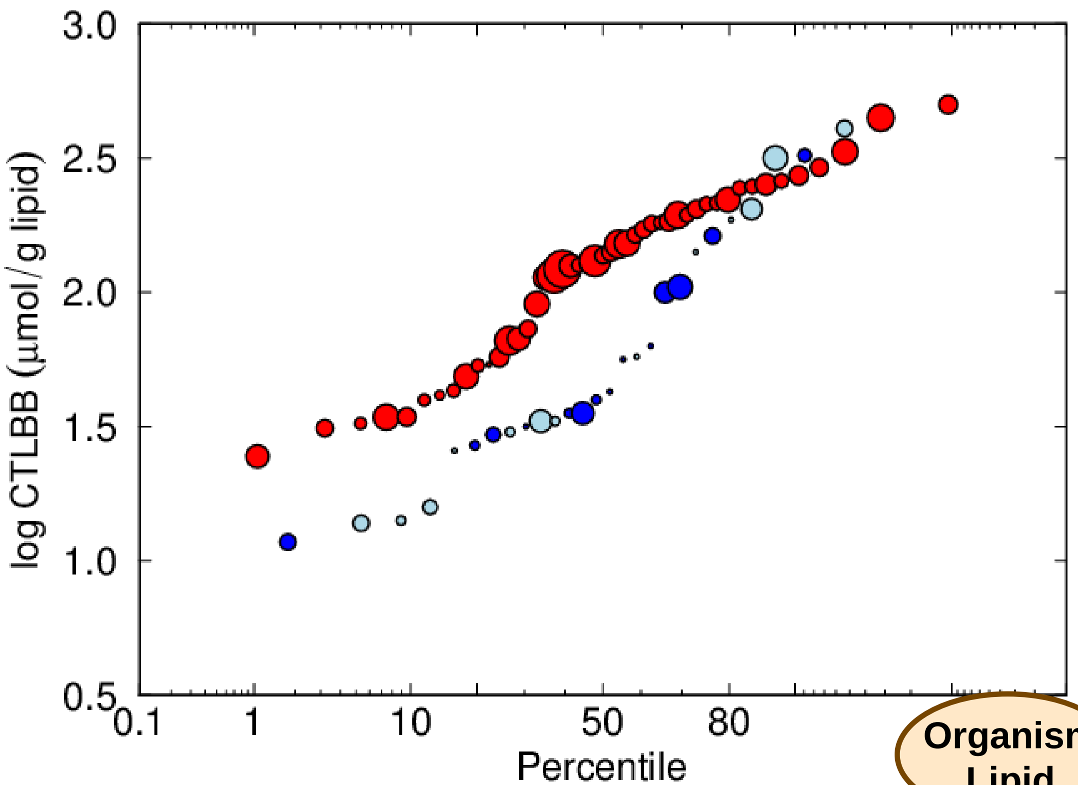
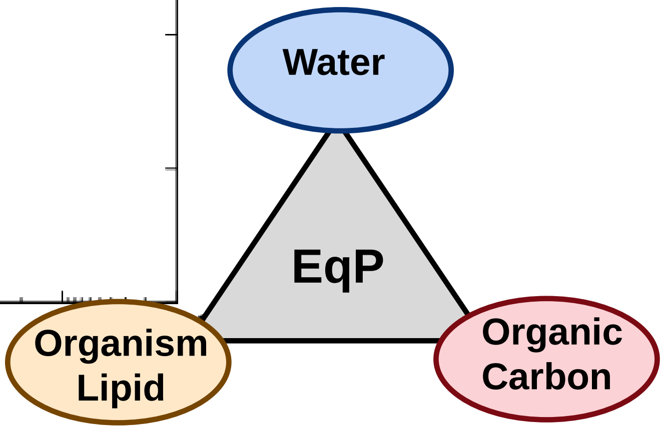
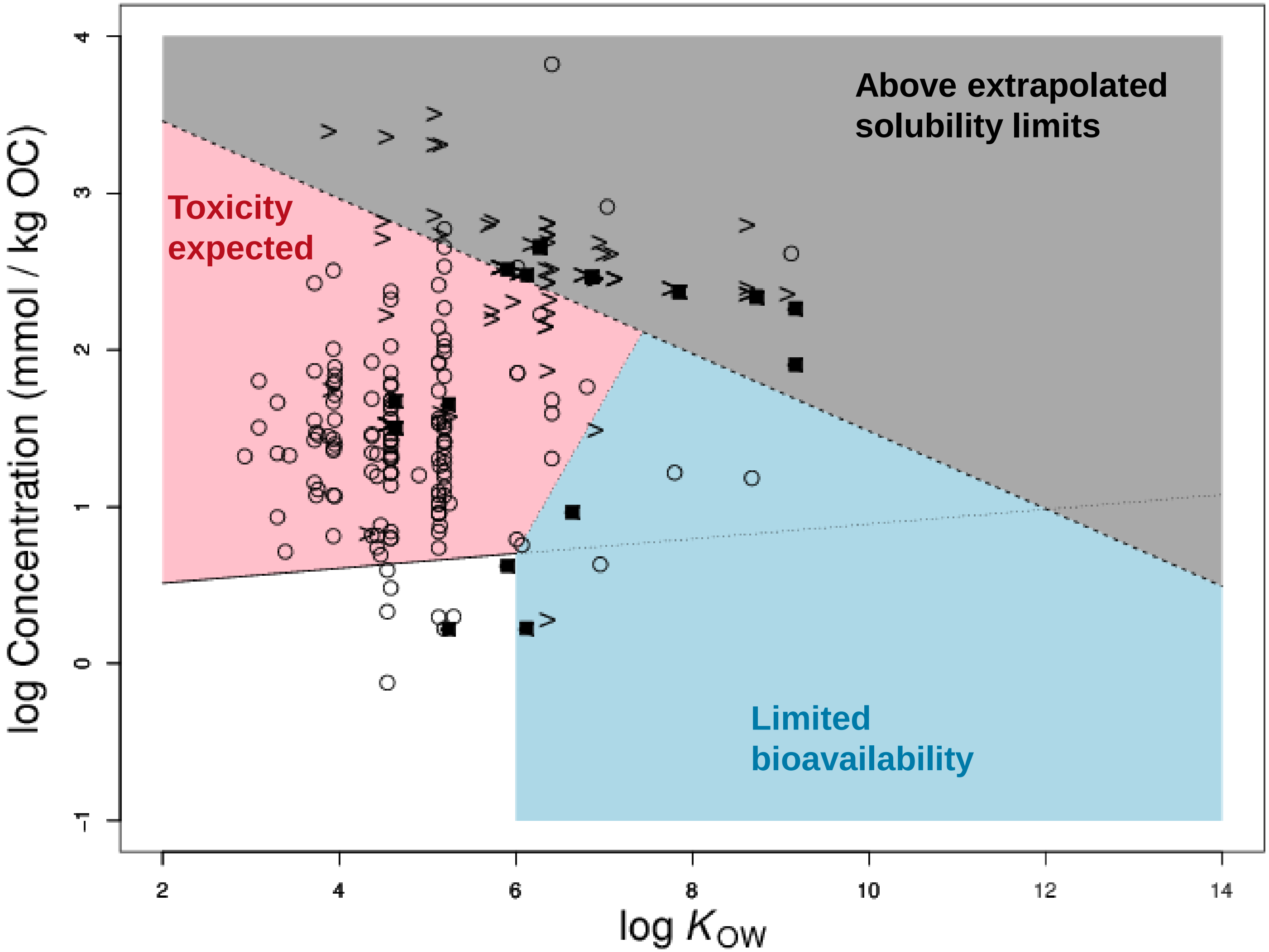




Validation of TLM-HC_5 using EqP

- HC_5 is protective of available chronic toxicity data: ~5% exceedance
- Conceptual model of soil bioavailability: substance concentration, logK_{OW}



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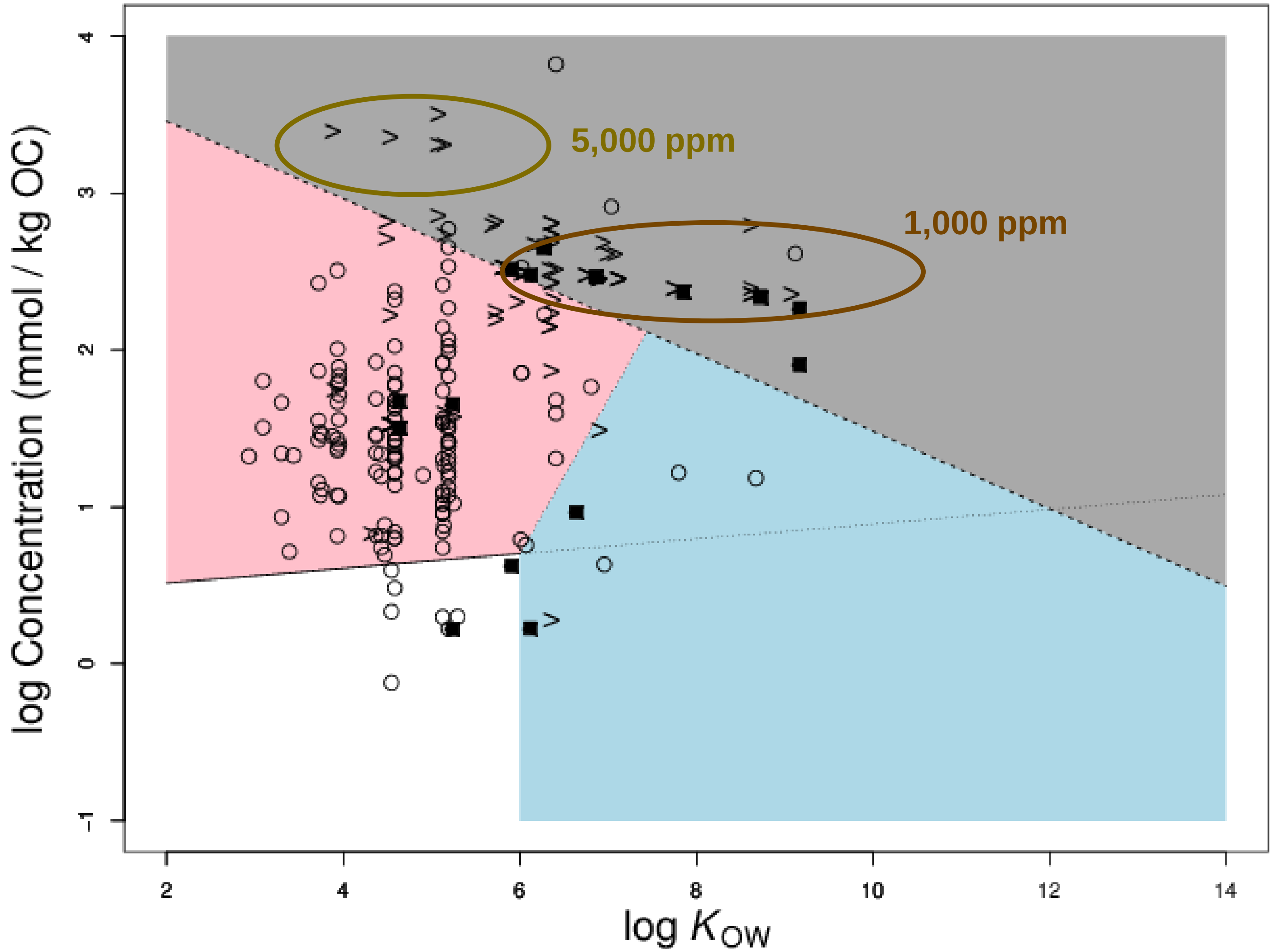
TLM-EqP framework informs test design

- Guidance often suggests testing at >1,000 ppm
  - Physical oiling is a confounding factor in this region
  - Conditioning and Aging of test material is important (EC 2004; Fuchsman et al 2006)



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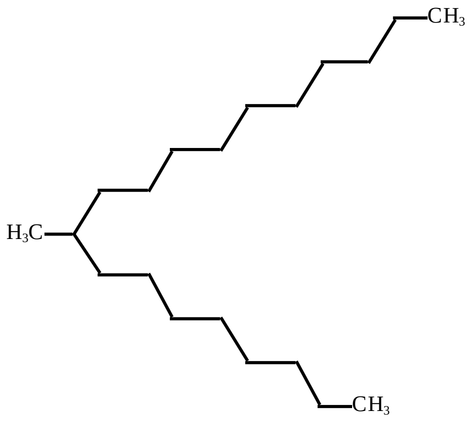
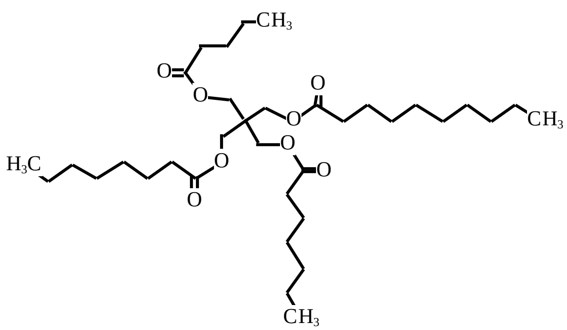
Case Study

- Hydrogenated Polyalpha Olefin (PAO)
  - Synthetic hydrocarbon engine oil
    - C20-22 alkanes
    - logK_{OW} **10-12**
    - Solubility < 0.001 µg/L



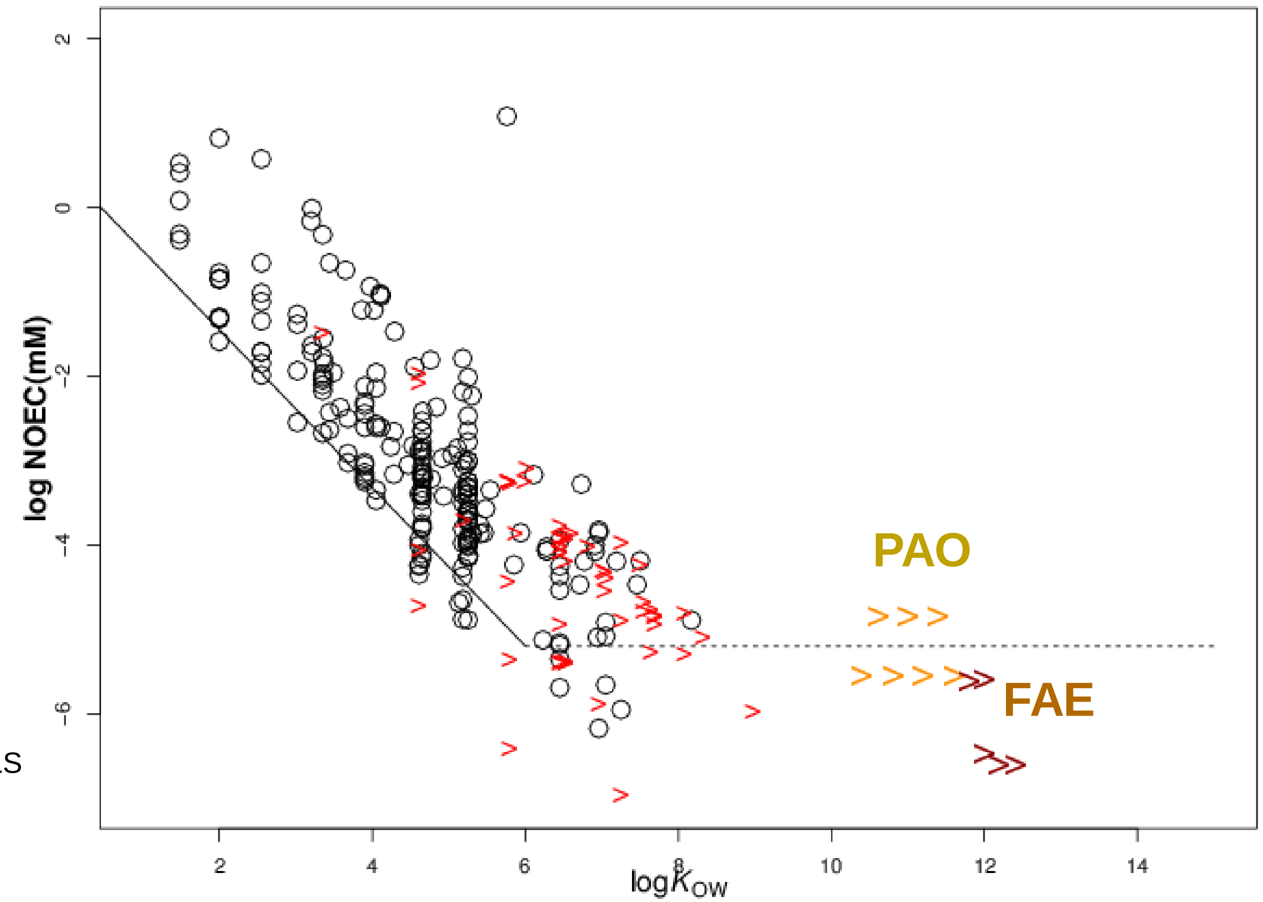
- Fatty Acid Ester (FAE)
  - Synthetic ester lubricant
  - C35 FA ester
  - logK_{OW} **~12**
  - Solubility < 0.001 µg/L



Available aquatic test data

- PAO and FAE are very insoluble
- Correspondingly, acute and chronic testing with fish, invertebrates and algae in water-only tests indicate no aquatic toxicity
- Substances are consistent with TLM framework

Acute: algae, fish, inverts
Chronic: Algae, inverts, ELS fish



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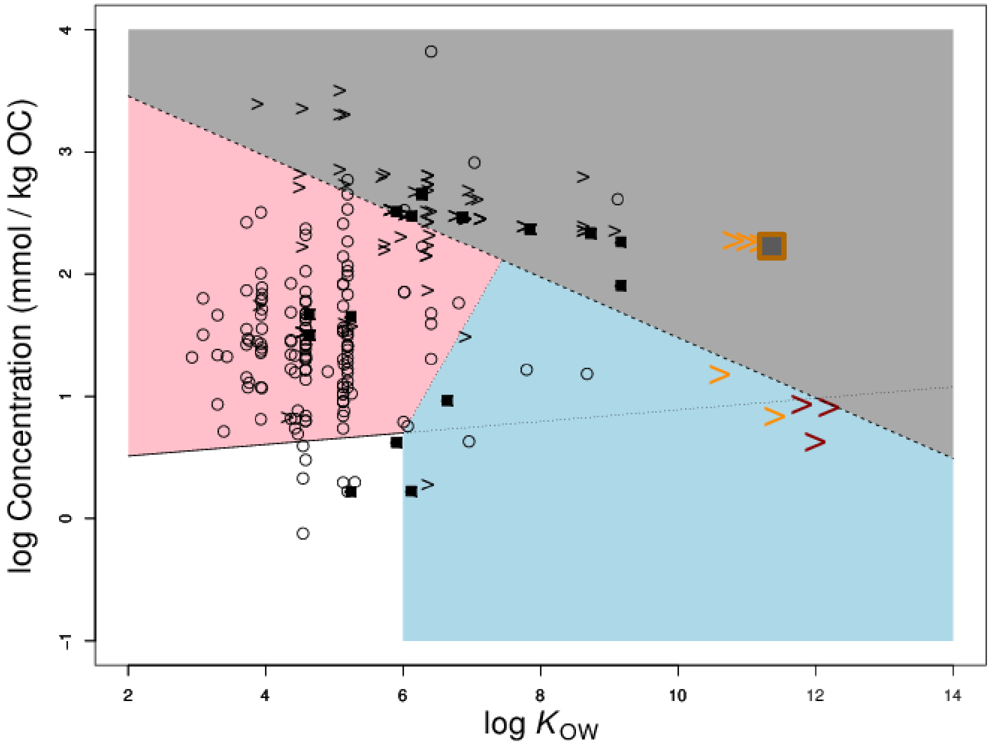
Available soil and sediment test data

- Consistently these materials are nontoxic to soil and sediment organisms (invertebrates, plants, microorganisms)
  - Initial testing indicated some effect on Radish
    - No aging, no conditioning
  - Above solubility limit
  - Likely confounded by physical oiling and does not reflect inherent toxicity
    - Analogous to aquatic testing above solubility



- Sed: *L.variegatus*,
- Soil: wheat, bean, radish, worm, microorganisms

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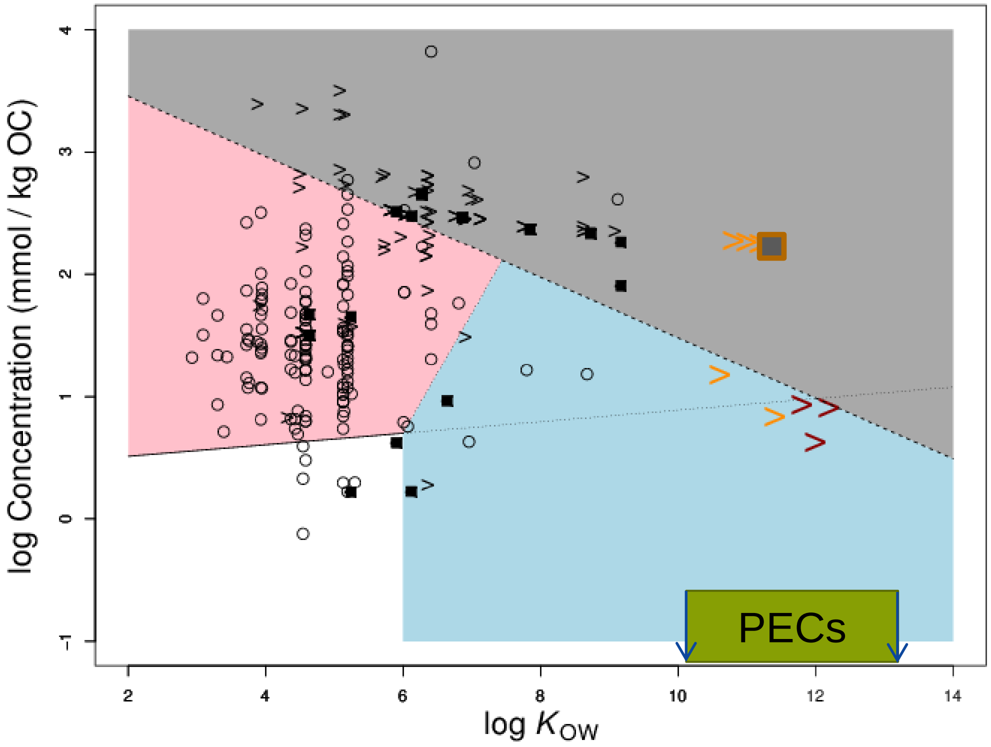
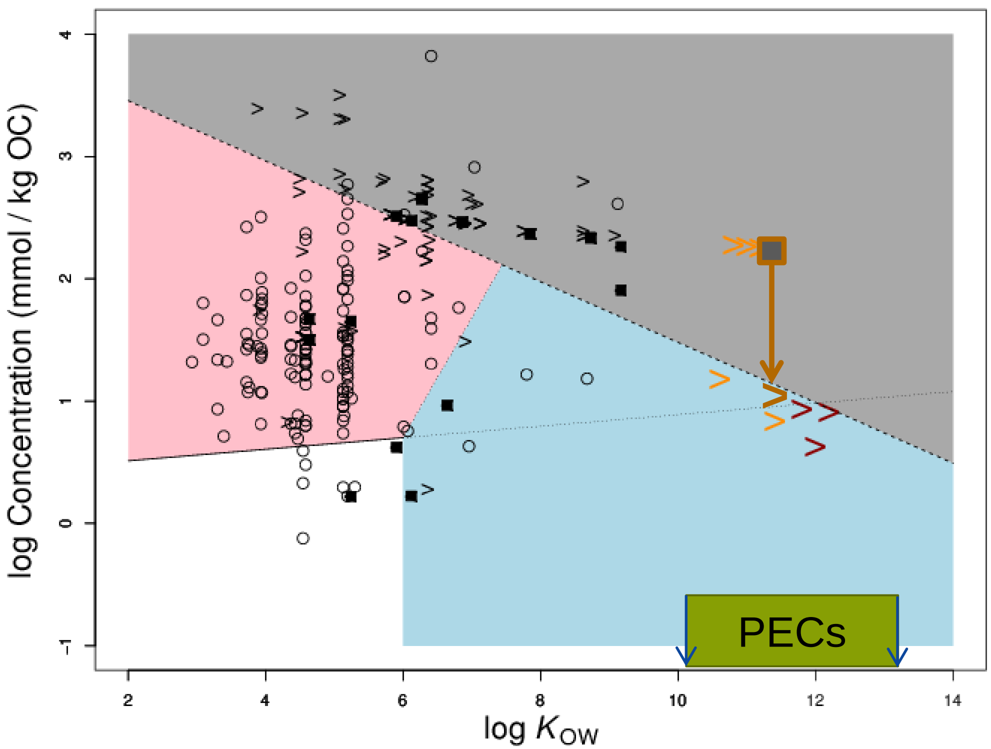
Available soil and sediment test data

- Integrated testing strategy developed to use results of Exposure Assessments (e.g., PECs) to inform Testing
  - PEC << PNEC and Solubility limit
  - More realistic testing limits needed to avoid artifacts associated with soil exposures to neat test substance
  - 100 ← 1000 ppm



Available soil and sediment test data

- Re-test (with 7-d aging, 3-d condition) confirms lack of toxicity of substance
  - Testing consistent with likely exposure
  - PECs < solubility
  - Oily phase material not expected to occur with aging at this treatment level



Conclusions

- TLM-EqP framework provides
  - improved mechanistic understanding test species sensitivity across media for a wide range of nonionic substances
  - pragmatic technical basis for designing and interpreting ecotoxicity testing programs for these substances

- Conducting soil toxicity tests with very hydrophobic test substances at elevated concentrations that exceeds the solubility in porewater may yield artifacts that do not accurately characterize soil hazard

- To avoid the confounding influence of potential physical effects, soil/sediment tests should be performed at lower upper-bound test exposures, i.e. conduct limit studies at ca. 100 ppm

Citations

- Environment Canada. 2004. Biological test method: test for toxicity of contaminated soil to earthworms (*Eisenia andrei, Eisenia fetida, Lumbriculus terrestris*). Report EPS 1/RM/43.
  http://publications.gc.ca/collections/collection_2013/ec/En49-7-1-43-eng.pdf

- HDR. 2015. Update of Target Lipid Model.

- McGrath JA, Di Toro DM. 2009. Validation of the target lipid model for toxicity assessment of residual petroleum constituents: monocyclic and polycyclic aromatic hydrocarbons. *Environ Toxicol Chem* 28:1130-1148

- Redman AD, Parkerton TF, Leon Paumen M, McGrath JA, den Haan K, Di Toro DM. Extension and validation of the target lipid model for deriving predicted no-effect concentrations for soils and sediments. *Environ. Toxicol. Chem.* 33:2679-2687

- Fuchsman PC, Barber TR, Lawton JC, Leigh KB. 2006. An evaluation of cause-effect relationships between PCB concentrations and sediment toxicity to benthic invertebrates. *Environ. Toxicol. Chem.* 25:2601-2612

Thank you!