Impacts of Low Levels of Residual Oils

# Predicting the Acute and Chronic Toxicity of MAHs and PAHs

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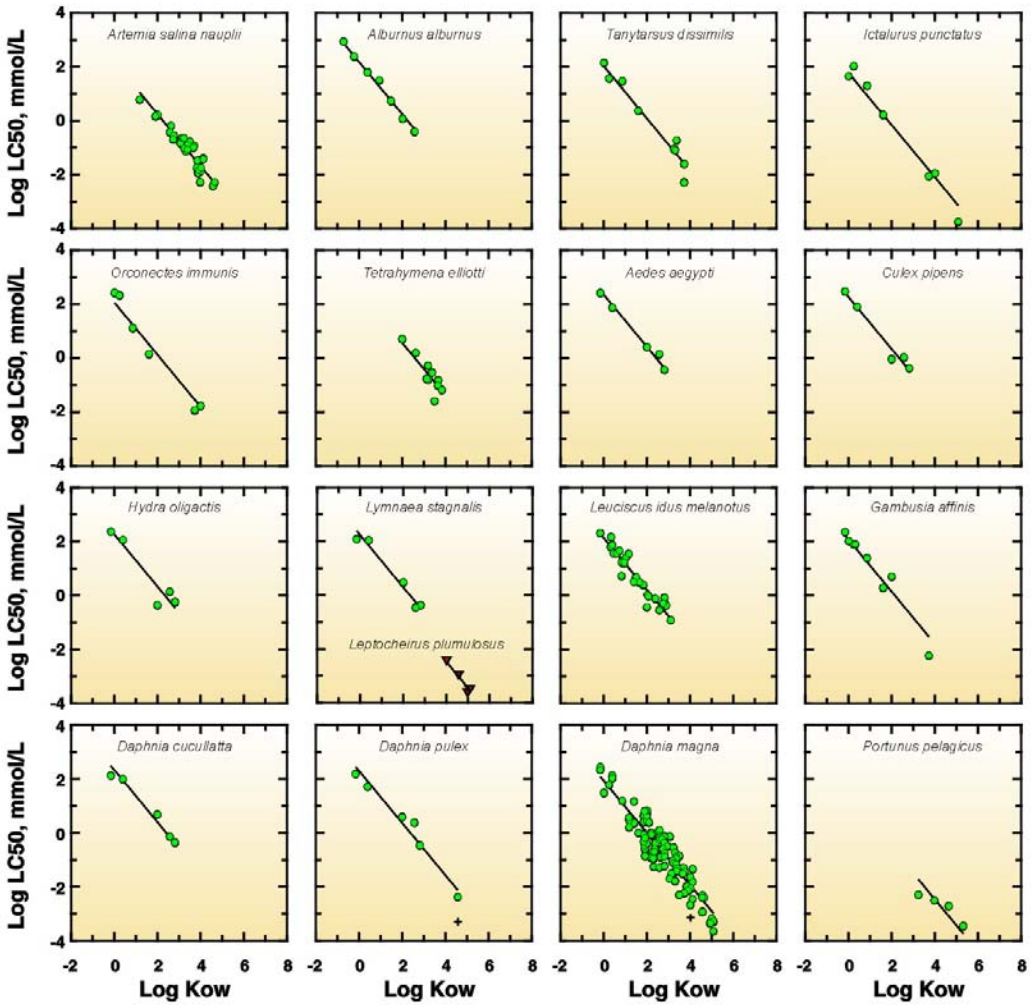
NOAA National Oceanic and Atmospheric Administration U.S. Department of Commerce

# Main Objectives

1. Identify key components of residual oil that contribute to toxicity
2. Establish a universal endpoint that can be applied across different oil sources
3. Derive endpoints for oil-related compounds that are protective of aquatic and benthic species from long-term sub-lethal effects

- Toxicity Model is Target Lipid Model (TLM)
- Not Suggesting chronic toxicity of compounds is via narcosis

# Acute Toxicity QSARs for Narcotics




(Di Toro et al., ETC, 2000)

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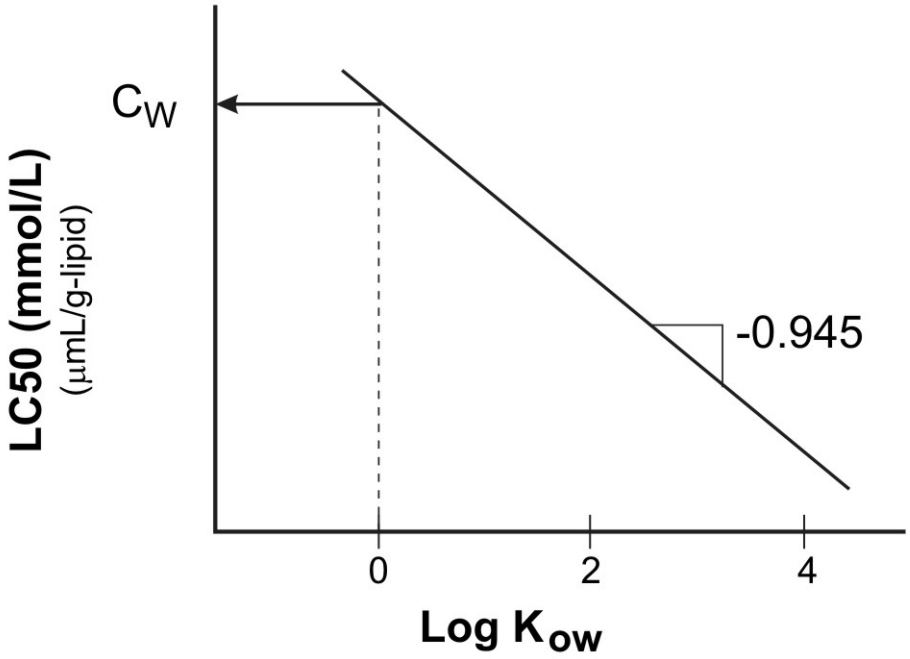
# Interpretation of Y-Intercept




$K_{ow} = 1$

$C_{OCTANOL} = C_w$

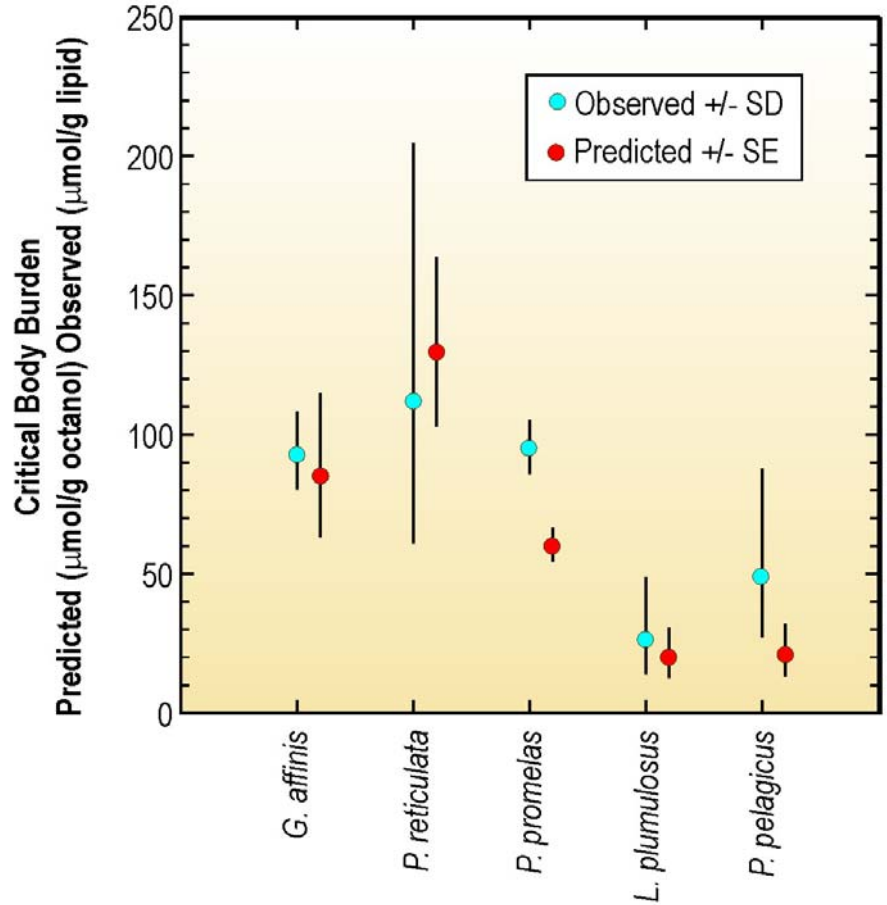
ASSUME: OCTANOL ~ LIPID

$C_{LIPID} = C_w$

$\therefore C_W$ = LC50 BODY BURDEN

(μmol/g-lipid)

# Comparison of Observed and Predicted Body Burdens




(Di Toro et al., ETC, 2002)

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# Computation of Water-only Effect Concentration

$$Log\ (C_W^*) = -0.945\ log(K_{OW}) + log\ (C_L^*) + cc$$

$C^*$ = Species specific critical target lipid body burden, $\mu mol/g_{octanol} = \mu mol/g_{lipid}$ $\mu mol/g_{lipid}$

$cc$ = Chemical class adjustment, -0.263 for PAHs

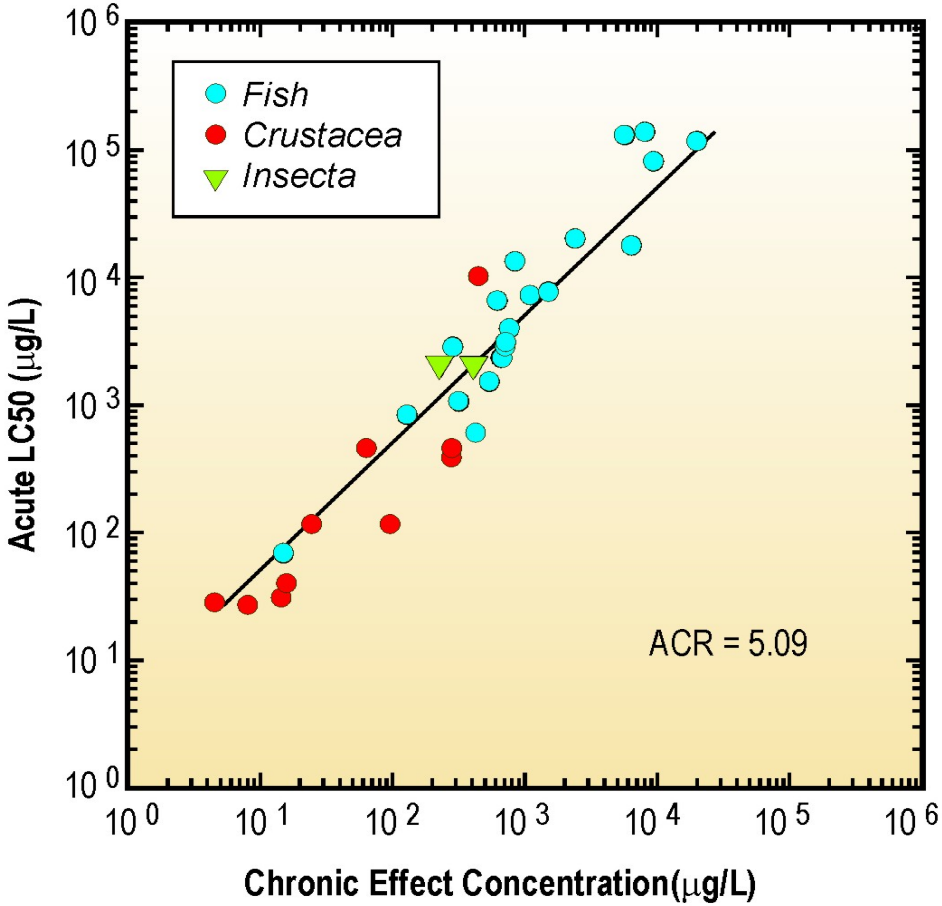
$C_W^*$ = Acute water-effect concentration, mmol/L

$$C^*, chronic = C^*, acute$$

$$acute_W \qquad \frac{W}{ACR}$$

$$ACR$$

# Determination of ACR




*(Di Toro et al., ETC, 2000)*

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# Normalization of Water Concentration

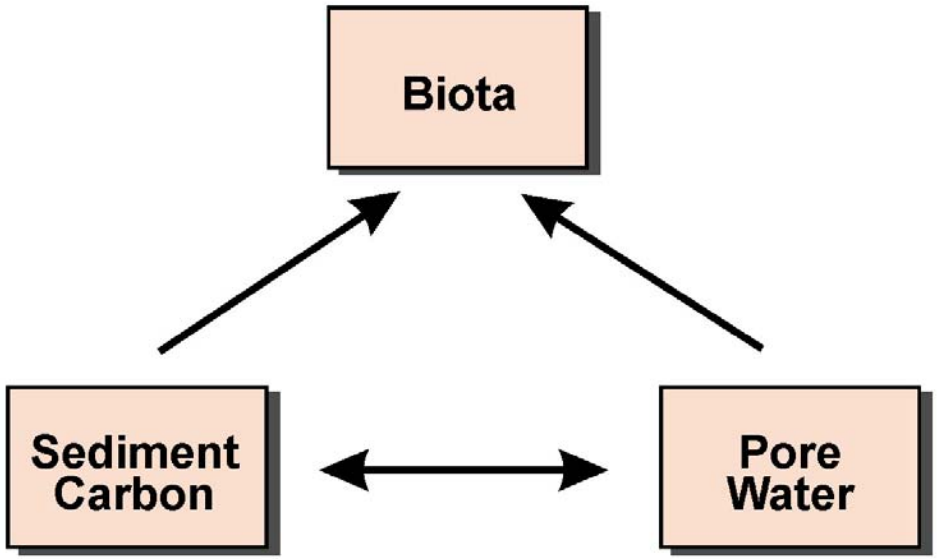
$$TU = \frac{\text{Measured Chemical Concentration in Water, mmol/L}}{C_w^*, \text{ mmol/L}}$$

$$TU_{mixture} = \Sigma TU$$

Theoretically $TU \geq 1$ Toxicity predicted

| | |
|---|---|
| $TU < 0.3$ | Toxicity Unlikely |
| $TU > 2.0$ | Toxicity Likely |
| TU between 0.3 and 2.0 | Toxicity Uncertain |

# Sediment-Pore Water Exposure




***Equilibrium Partitioning***

*(Di Toro et al., 1991)*

# Organic Carbon Normalized Sediment Effect Concentrations

$$C^{*}_{OC} = K_{OC} \times C^{*}_{W}$$

$\mu g/kgOC$ $\quad L/kgOC$ $\quad \mu g/L$

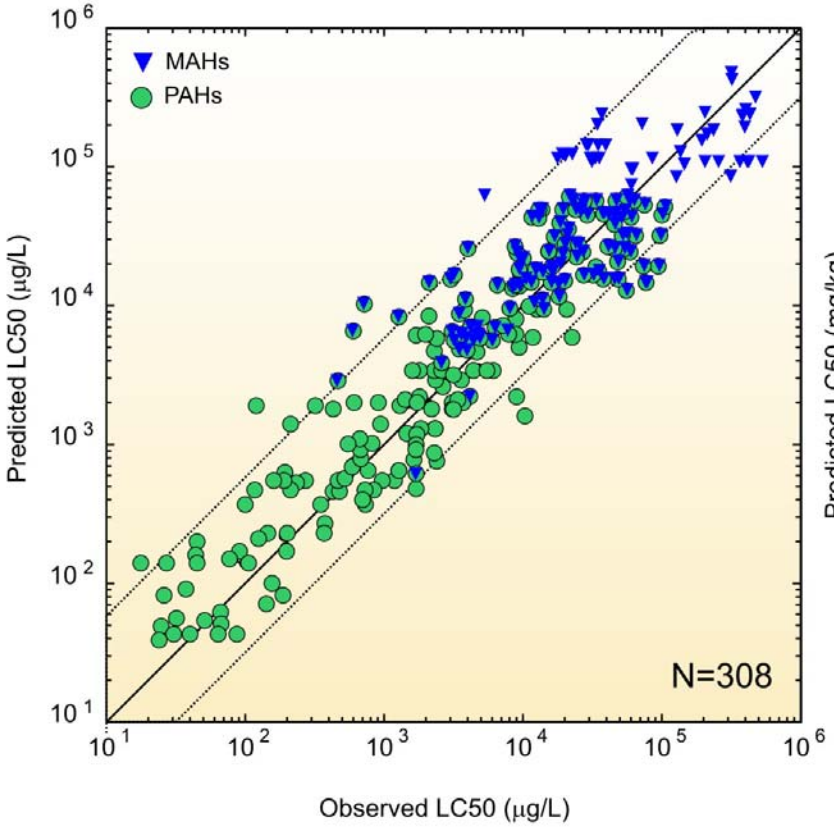
$$TU = \frac{\text{Measured Chemical Concentration, } \mu g/K_{gOC}}{C^{*}_{s,OC}}$$

# Literature Summary

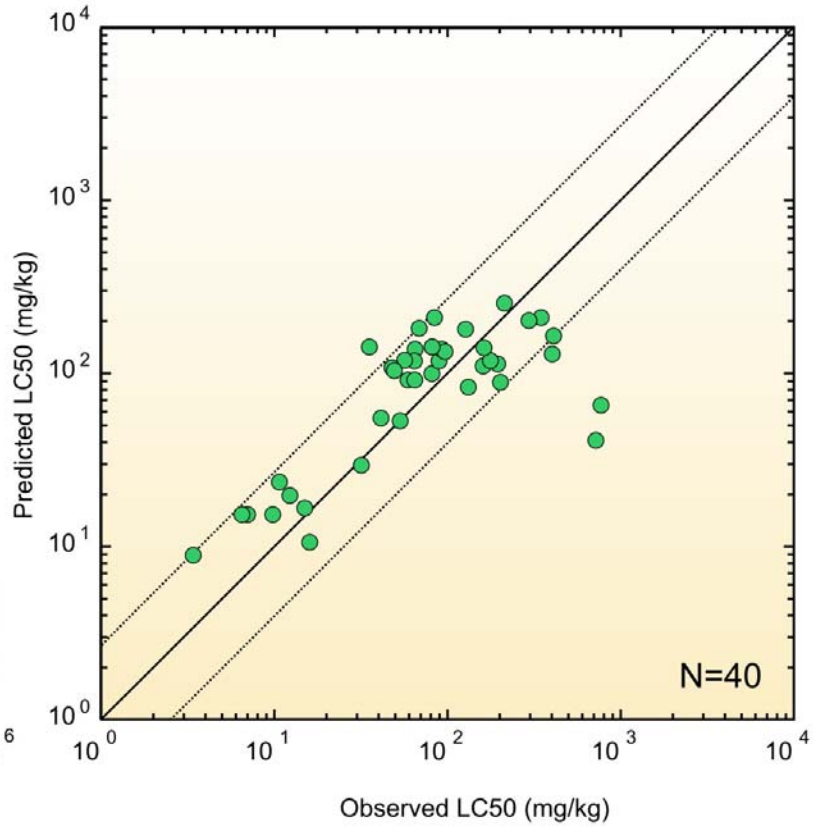
| | References Reviewed | References Accepted |
|---|---|---|
| Water Column | 141 | 80 |
| Sediment | 64 | 21 |
| TOTAL | 205 | 101 |

# Acute Effects (lethality) - Single Exposures

## Water Column




## Sediment

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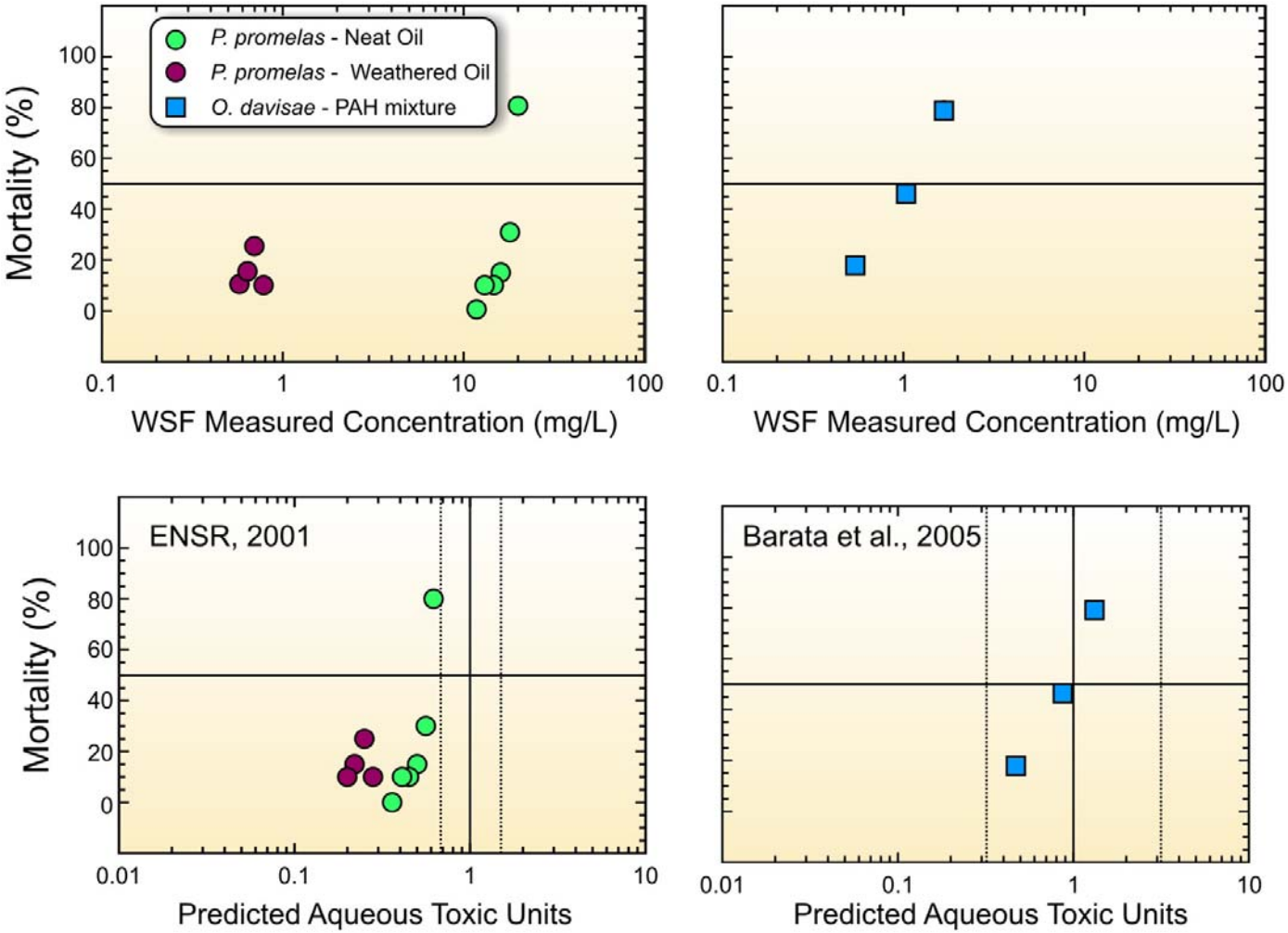
# Water Column – Acute Effects
# PAH Mixtures



# 90% Confidence Limits in Predicted Effect Concentration

$$\log(HC_5) = E(m)\log(K_{ow}) + E\{\log(C_L^*)\} - E\{\log(ACR)\} - k_Z\sqrt{V\{m\}\log(K_{OW})^2 + V\{\log(ACR)\} + V\{\log C_L^*\}}$$

$$\log(HC_5) \qquad + k_Z\left[\sqrt{\qquad\qquad}\right]$$

**Where:**

$HC_5$ = aqueous concentration that protects 95% of organism (mmol/L)

$E\{m\}$ = universal narcosis slope, -0.945

$E\{\log(C_L^*)\}$ = log mean CTLBB mmol/g $_{octanol}$

$E\{\log(ACR)\}$ = log mean acute to chronic ratio.

$k_Z$ = 95% confidence sample-size-dependent extrapolation factor,

$V\{m\}\log(K_{OW})$ = variance of universal narcosis slope

$V\{\log(ACR)\}$ = variance of log (ACR)

$V\{\log C_L^*\}$ = variance of log CTLBB

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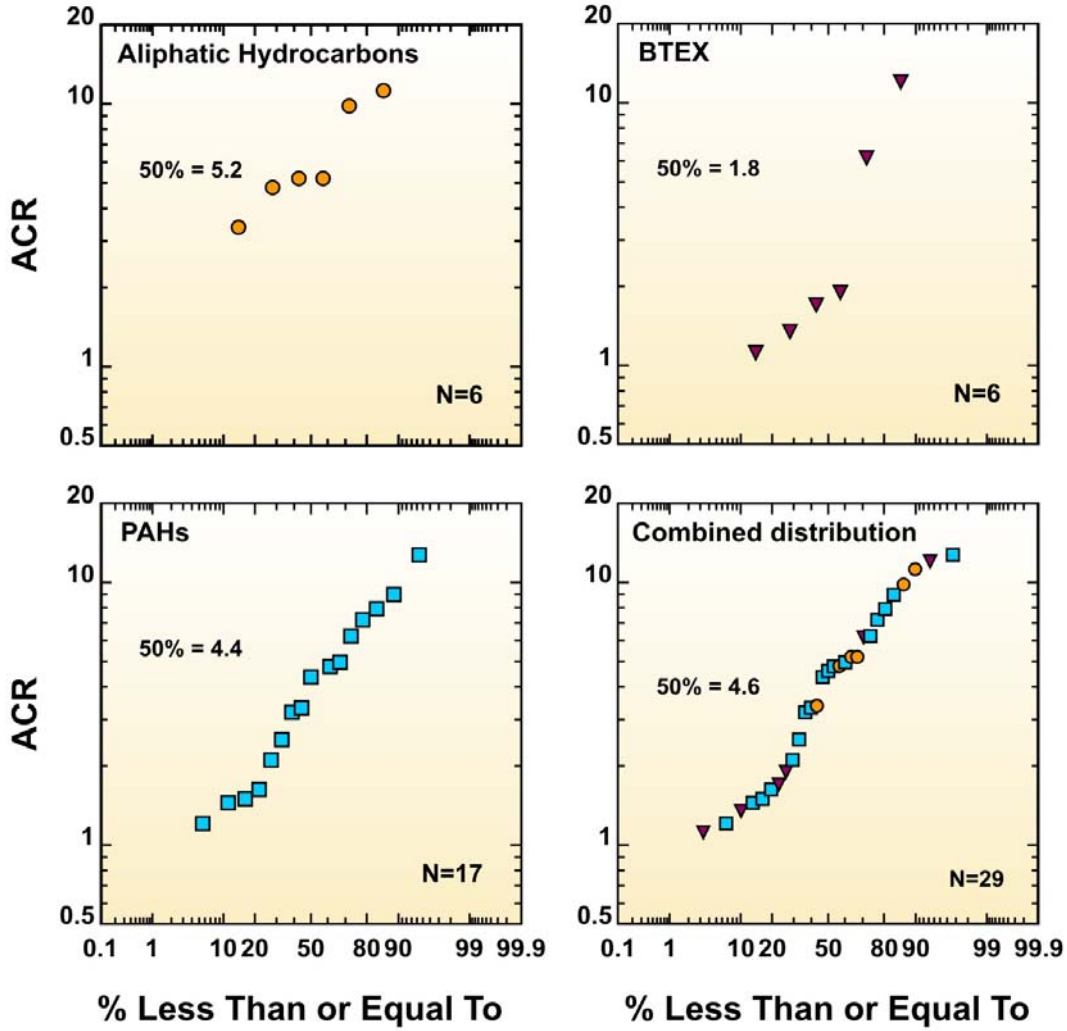
# Chronic Effects (Growth, Reproduction, Mortality) – Single Exposures

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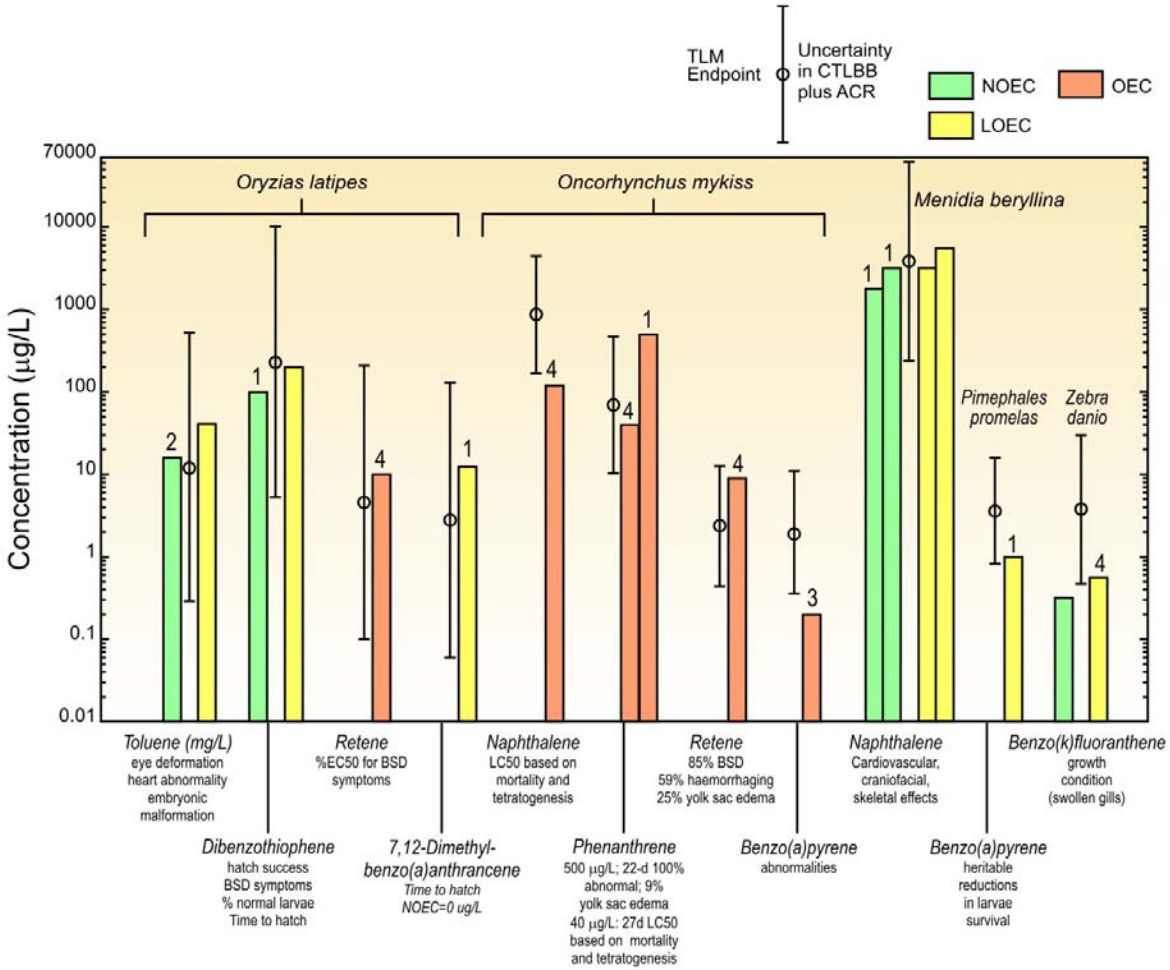
# Water Column – Other Chronic Sublethal Effects
# Single PAH Exposures

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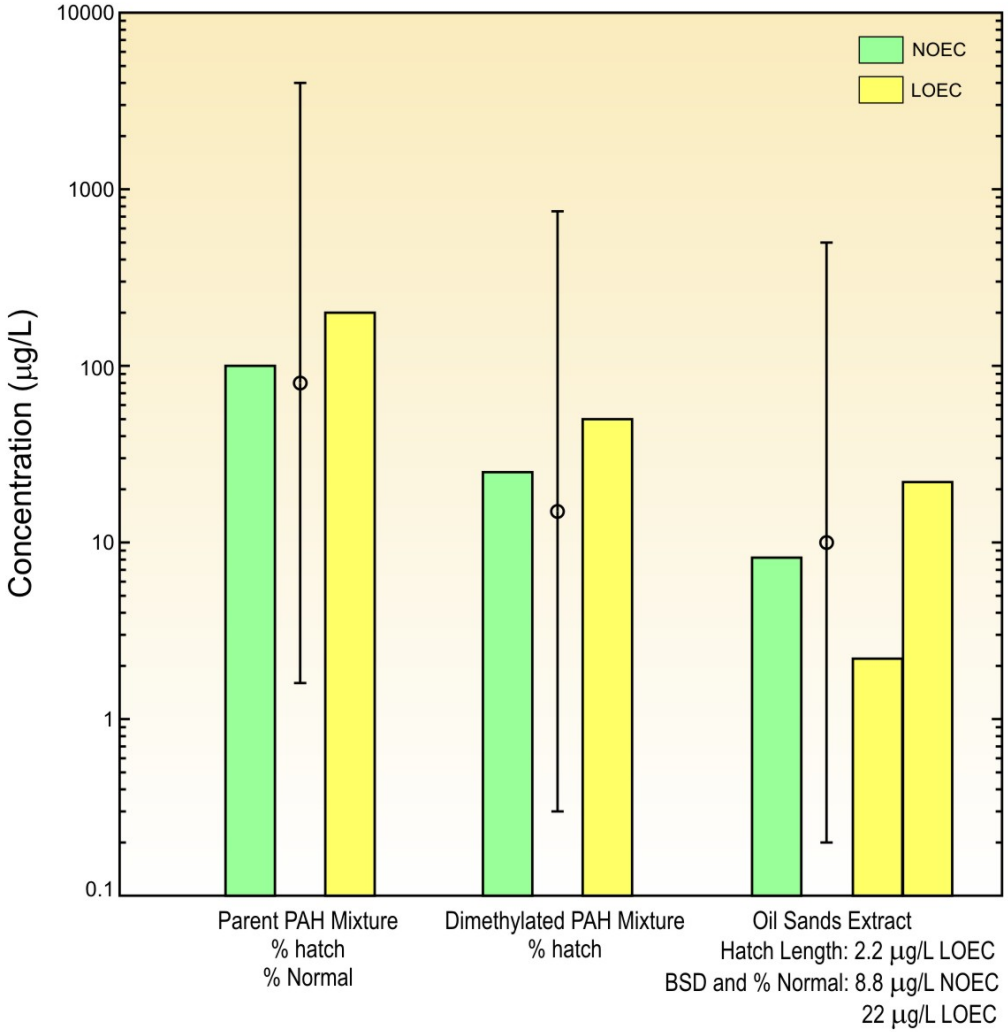
# Water Column – Other Chronic Sublethal Effects - PAH Mixtures

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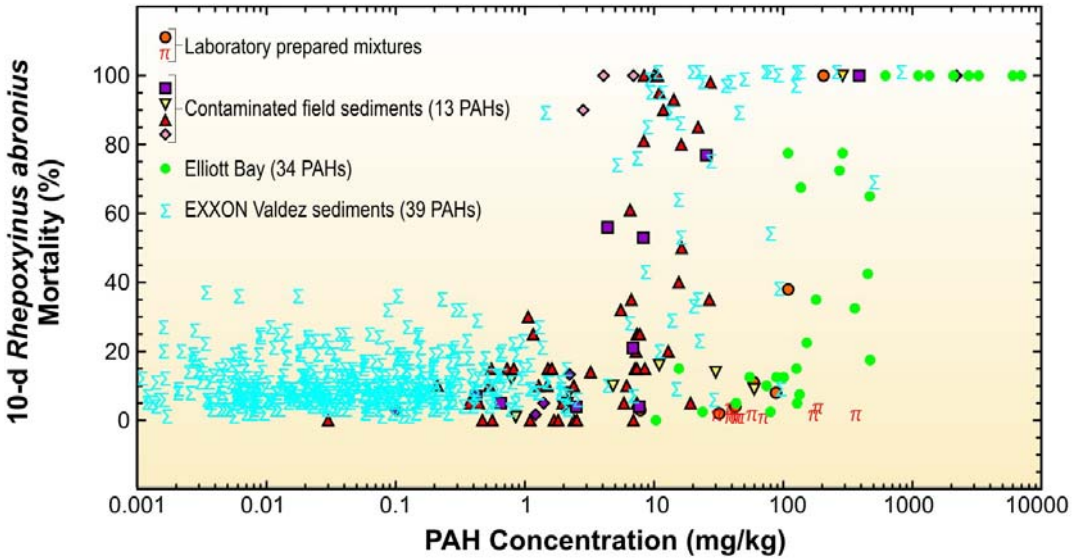
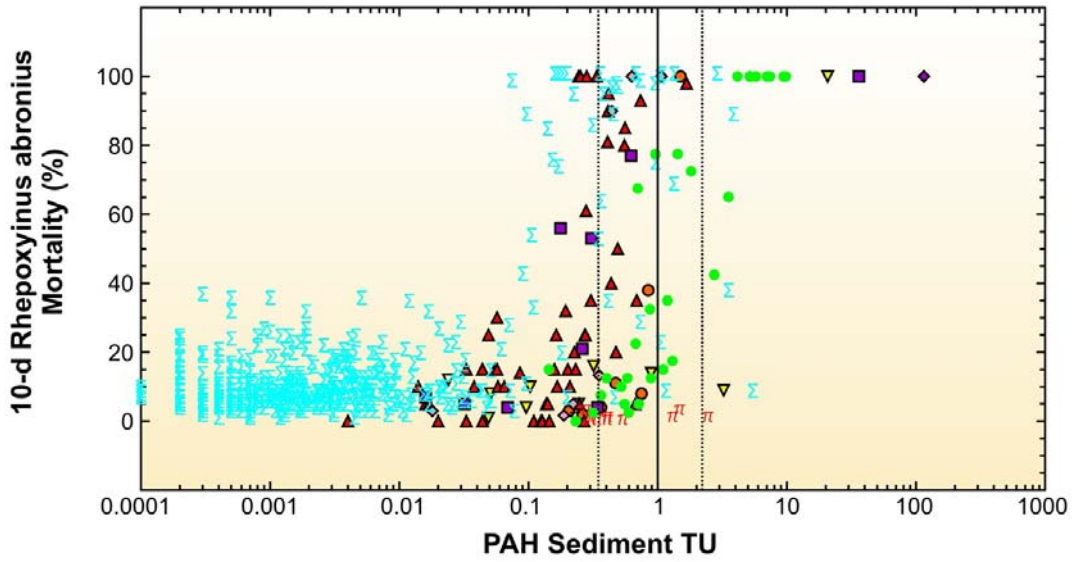
# Sediment – Acute Effects - PAH Mixtures

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# Derivation of HC5 Values That Protect 95% of Species

$$\log (HC_5) = E(m) \log (K_{ow}) + E\{\log (C_L^*)\} - E\{\log (ACR)\} - k_Z \sqrt{V\{m\}\log(K_{OW})^2 + V\{\log(ACR)\} + V\{\log C_L^*\}}$$

$E\{\log (C_L^*)\}$ = Geometric mean of all CTLBBs

$k_Z$ = Extrapolation constant based on number of ACRs

$V\{\log C_L^*\}$ = Variance of all CTLBBs

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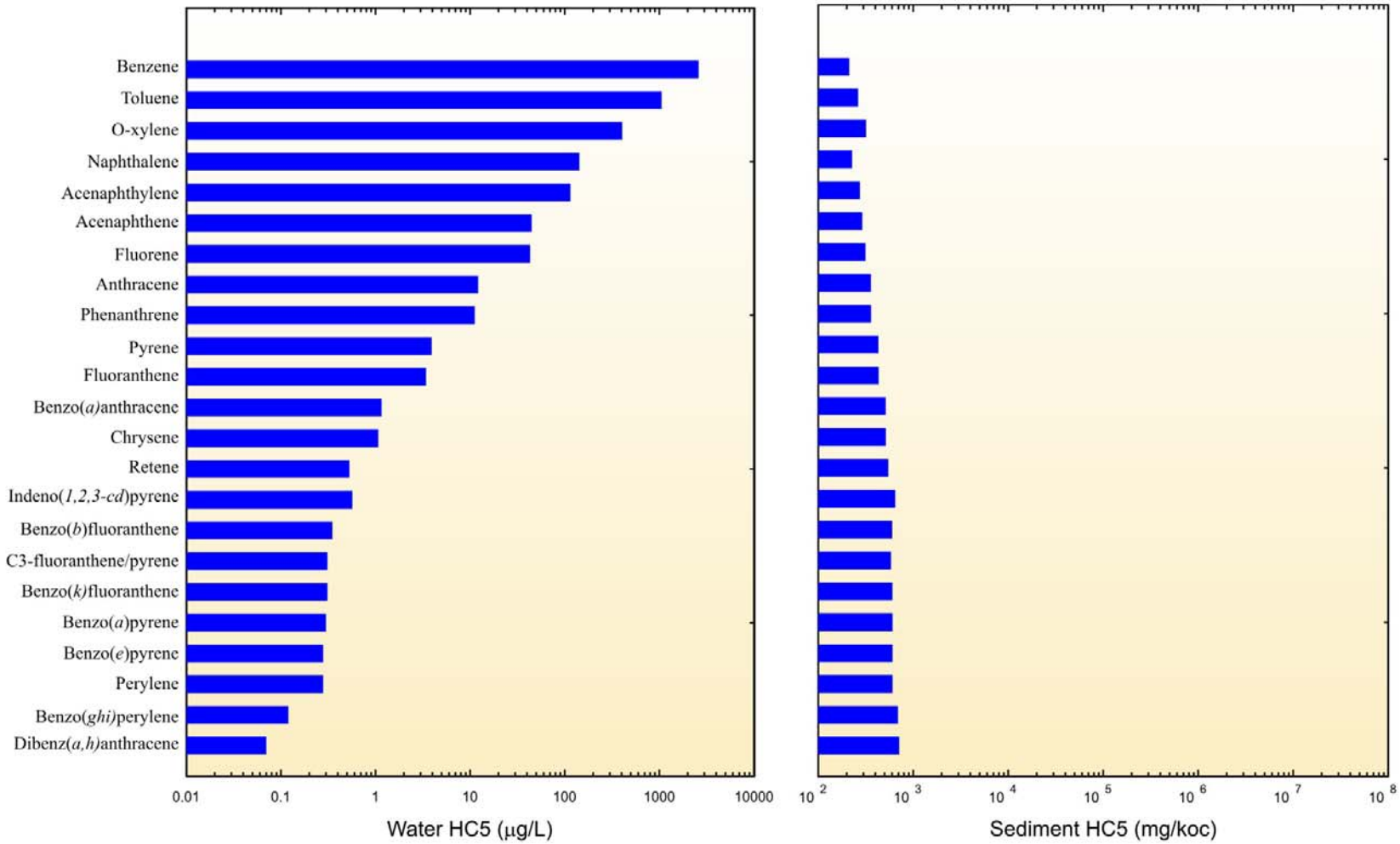
# HC5 Values for Water and Sediment

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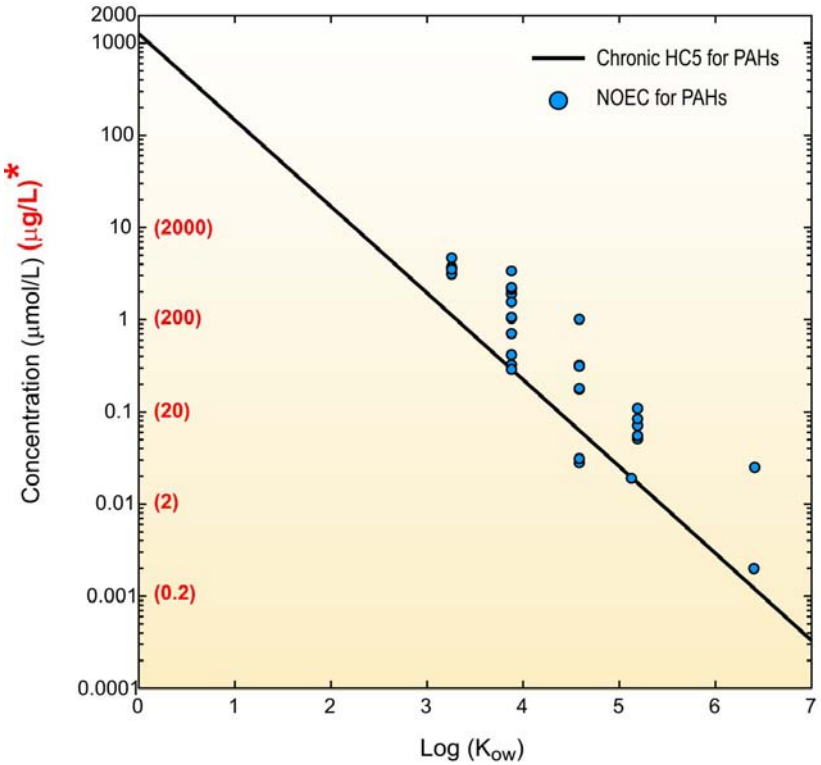
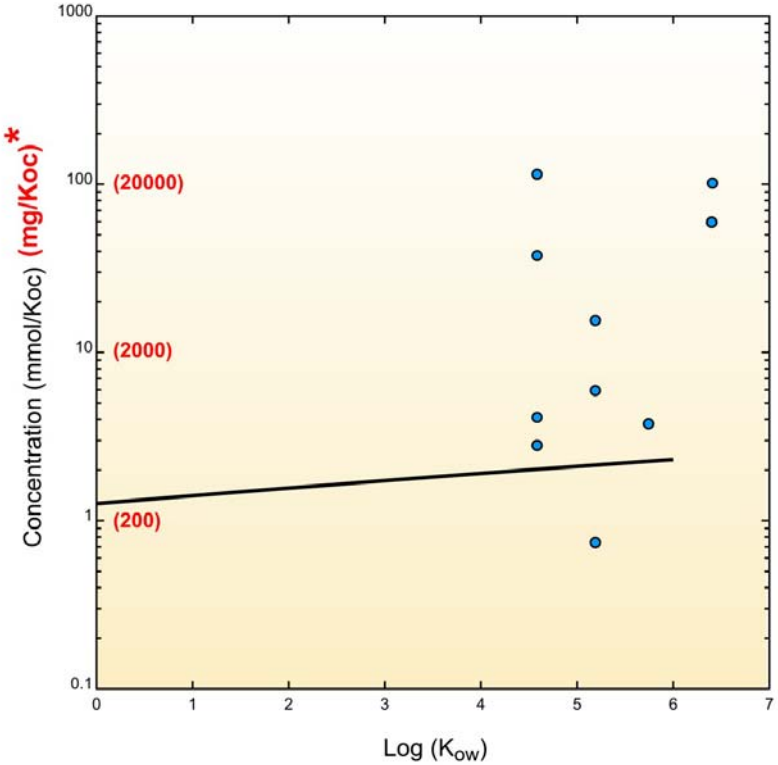
# Comparison of HC5s and NOECs for PAHs

## WATER




* Assuming Molecular Weight of 200g/mole

## SEDIMENT

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