INVESTMENTS IN EDUCATION DEVELOPMENT

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From passive sampling of sediment to lipid based concentrations

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Objectives

- To calculate ***equilibrium partitioning concentration*** in lipids ($C_{lipid\ partitioning}$) based on equilibrium passive sampling

- Comparison to actual measured lipid normalized concentrations in biota ($C_{lipid\ normalized}$)

Hypotheses

$$C_{\mathbf{free}} \leftrightarrow C_{\mathbf{passive\ sampler}} \leftrightarrow C_{\mathbf{biota\ lipids}}$$

$$C_{\text{lipid partitioning}} \approx C_{\text{lipid normalized}}$$

$$C_{\text{lipid partitioning}} < C_{\text{lipid normalized}}$$

$$C_{\text{lipid partitioning}} > C_{\text{lipid normalized}}$$

Coated glass method

- Several coating thicknesses (from 1 µm to 16 µm)
- Equilibration in laboratory

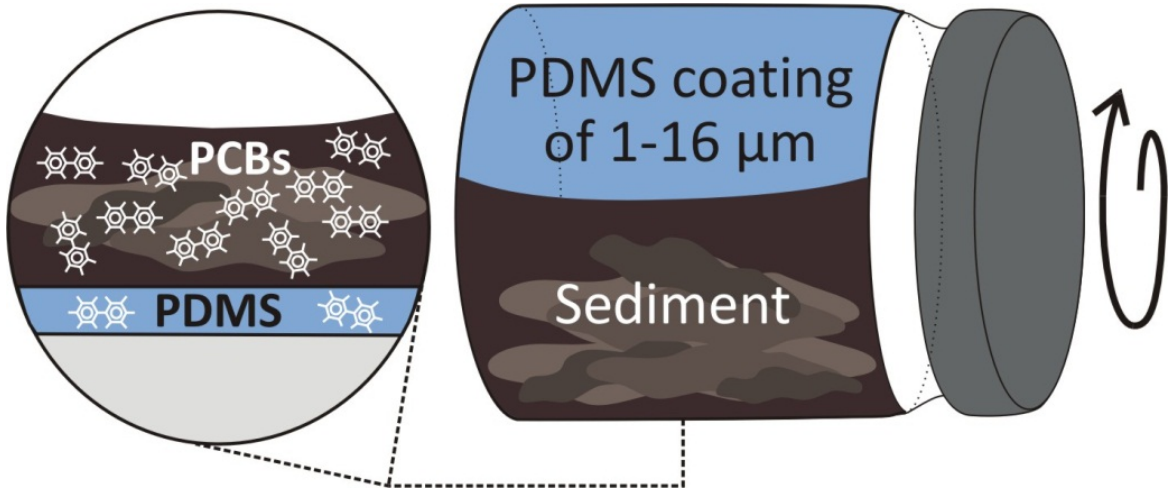
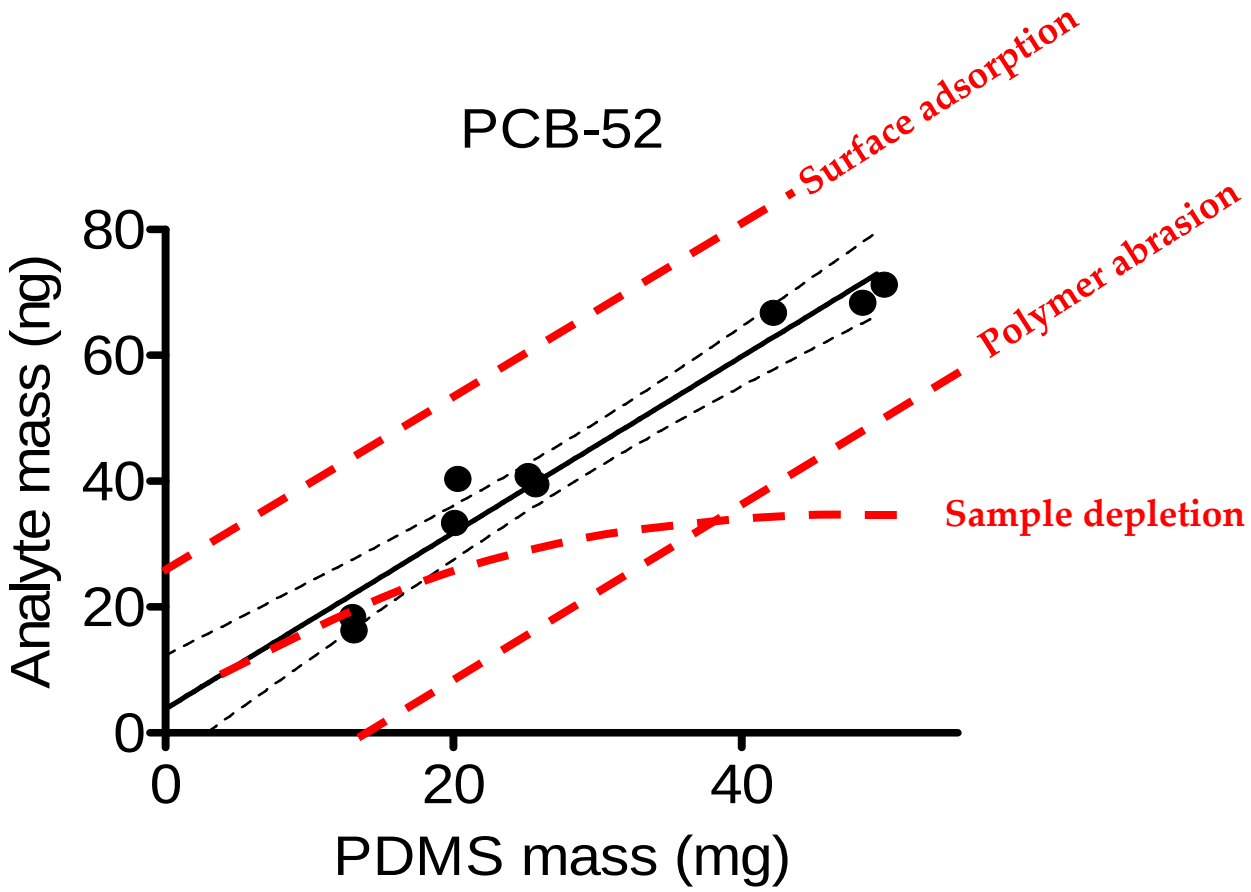


Fig. Annika Jahnke

Different coating thicknesses → Built-in QA/QC



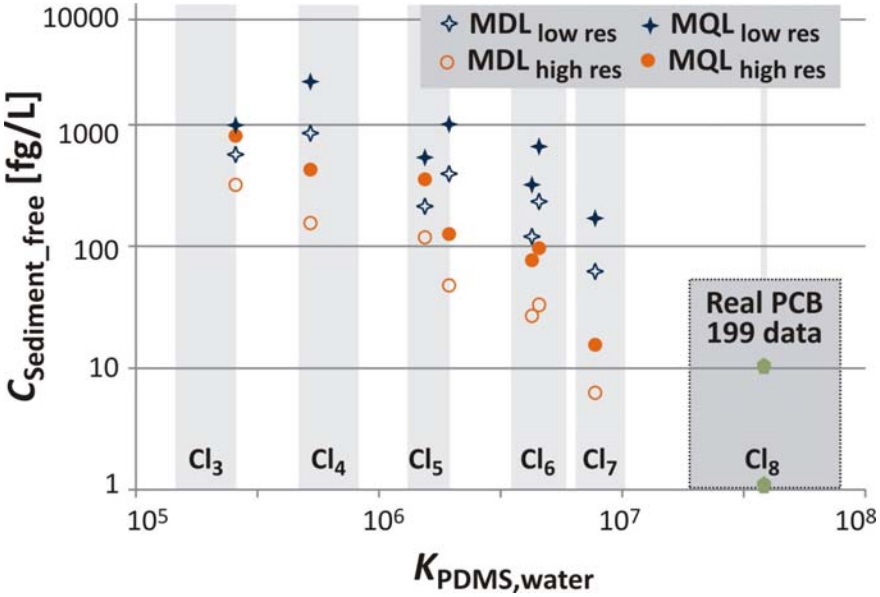
Reichenberg et al. 2008 *Chem. Central J., 2, 8.*

Method sensitivity test

- Method quantification limits (**MQLs**): average blank + 10 times the standard deviation

- For **7 indicator PCBs**:

	fg/L
GC/HRMS	**16-800**
GC/LRMS	**168-2250**



Jahnke et al. 2012 Environ Sci Technol 46

Calibration of coated glass analysis to $C_{lipid\ partitioning}$

$C_{lipid\ partitioning} = C_{passive\ sampler} * K_{lipid,passive\ sampler}$

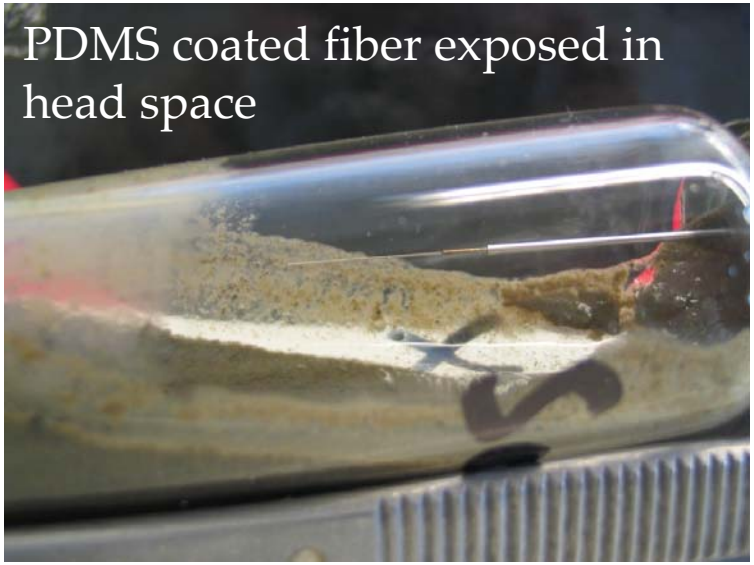
$K_{lipid,PDMS}$ have been published for PCBs:

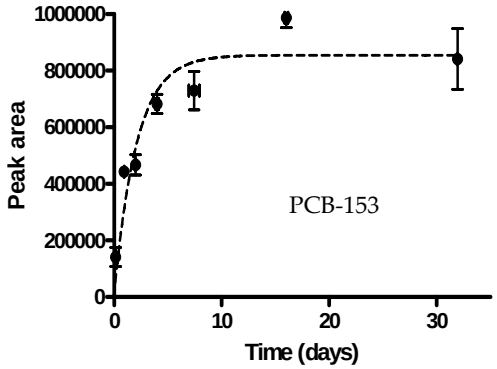
Jahnke et al. 2008. Chemosphere, 73, 1575–1581

Head space sampling
HS-SPME

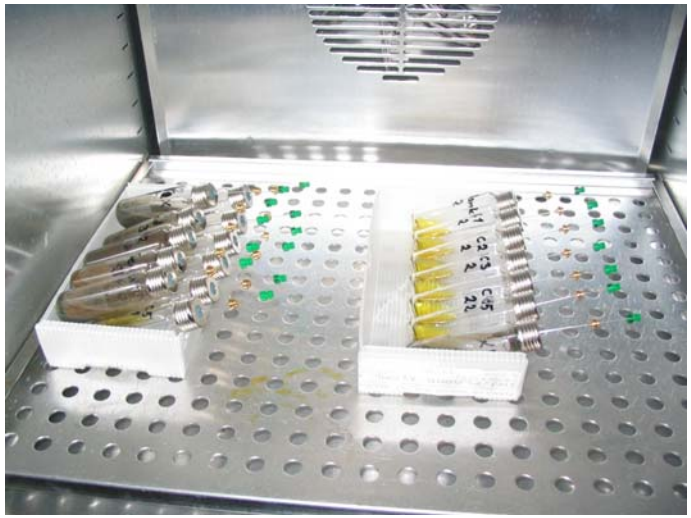
- SPME fiber is equilibrated with the sediment

- Time series analysis to determine C_{fiber} at equilibrium

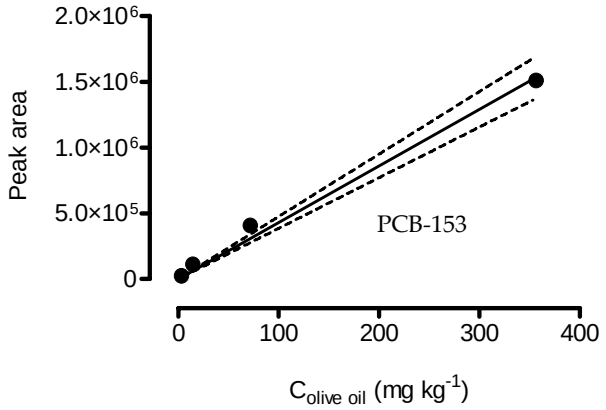




Calibration of HS-SPME



- External calibration standard in lipid (olive oil)
- Direct calculation of $C_{lipid,partitioning}$
- Benefits
  - Solvent free approach
  - Extraction and analysis can be manual or fully automated



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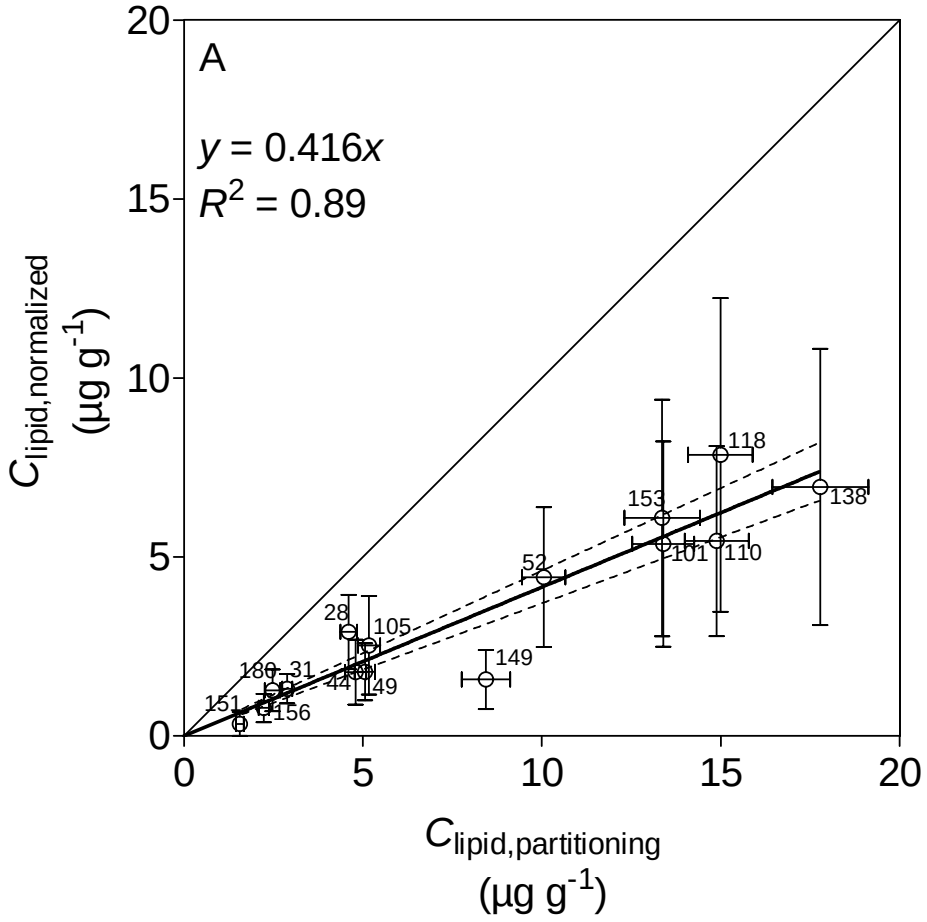
	Headspace-SPME	Coated glass
Working principle	Equilibration in head space and thermal desorption	PDMS coatings are equilibrated, extract injected on instrument
Calibration to $C_{lipid,partitioning}$	External calibration above spiked olive oil	$C_{lipid,partitioning} = C_{PDMS} * K_{lipid,PDMS}$
Special features	Applicable to dry samples	Combines thin coatings with high polymer mass
Confirmation of equilibrium	Time series measurements	Proportionality between mass of analyte and polymer (QA/QC)
Surface fouling	No physical contact with sample	Absence of artifacts indicated by the same proportionality

Mäenpää et al. 2011 Environ Sci Technol 45

$C_{lipid,normalized}$ vs. $C_{lipid,partitioning}$ Chironomidae larvae

- $C_{lipid\ partitioning}$ av. 2.4 times higher than $C_{lipid\ normalized}$



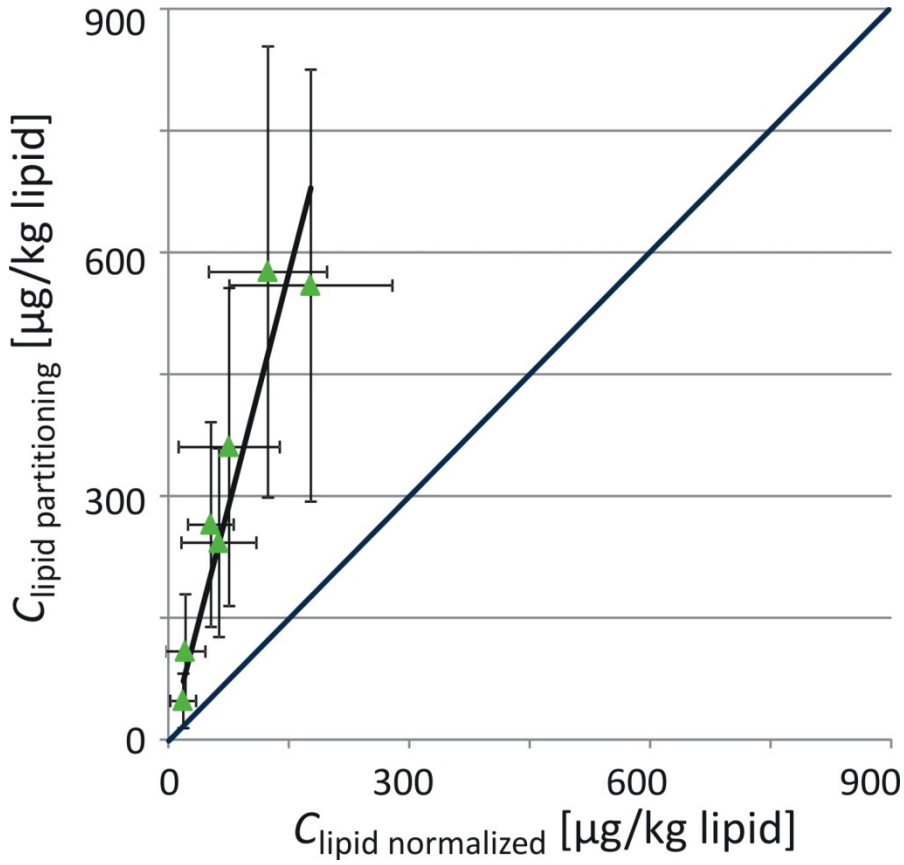
Mäenpää et al. 2011 Environ Sci Technol 45

Slide 11

A11 Seems as if Chironomidae are mosquito larvae, not worms?
AnnikaJahnke, 11/05/2011

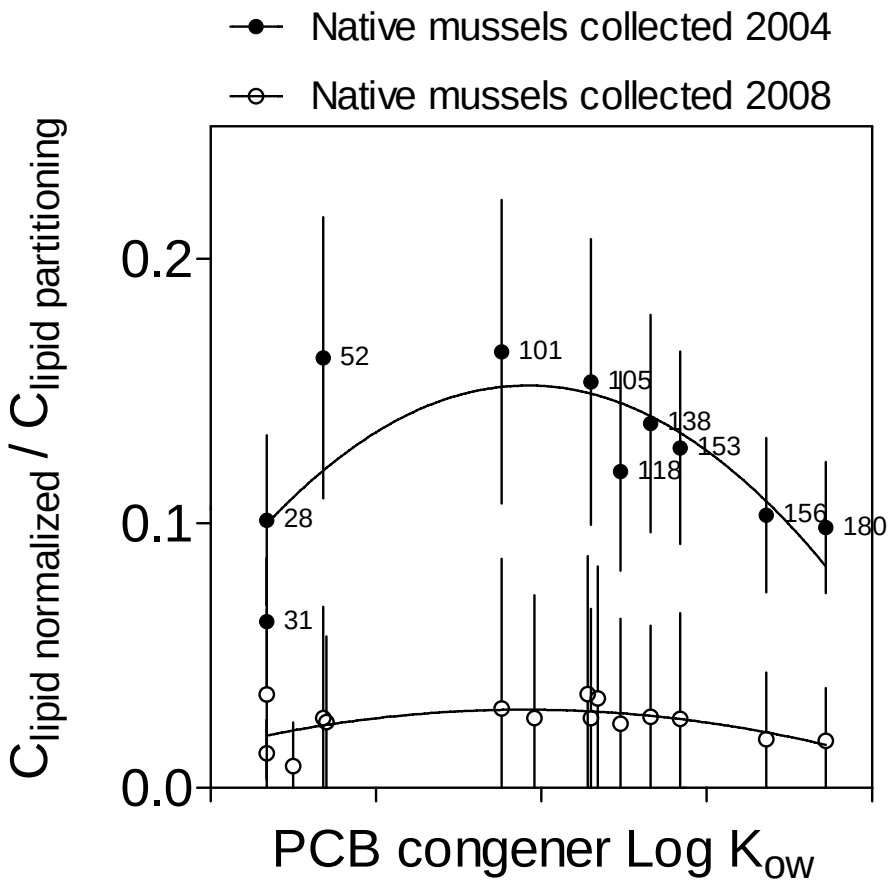
$C_{lipid\ partitioning}$ vs. $C_{lipid\ normalized}$ Native fish

- $C_{lipid\ partitioning}$ av. 5.2 higher than $C_{lipid\ normalized}$



Jahnke et al. 2012 Environ Sci Technol 46

$C_{lipid,normalized}$ vs. $C_{lipid,partitioning}$ Native mussels



Mäenpää et al. Manuscript in preparation

Conclusions

- Calibration with $K_{lipid,passive\ sampler}$
  - post measurement calibration
  - requires analyte and media specific K values

- Direct calibration using partition standards in lipids
  - complete calibration within one step
  - easier to apply for new chemicals and media

- $C_{passive\ sampler}$ can be converted to useful information to be used in environmental risk assessment

- $C_{lipid\ partitioning}$
  - predicts equilibrium level