Inter-calibrating passive sampling and dosing polymers

based on polymer-polymer partition ratios of PCBs, PAHs and organo-chlorine pesticides

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Equilibrium sampling & passive dosing

- $K_{polymer:water}$ required to determine $C_{free} = \frac{C_{polymer}}{K_{polymer,water}}$

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- $K_{polymer:water}$ not always available
- $K_{polymer:water}$ often limits accuracy & precision
  - (1) experimental errors
  - (2) polymer:polymer partitioning differences

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  - **make data of different passive samplers sets comparable**
  - **connect passive sampling & passive dosing**
- **calibration of new polymers**
  - **monitoring with new polymeric materials of unknown $K_{polymer,water}$**

Calibration

$$\log K_{pol.y,medium} = \log K_{pol.x,medium} + \log K_{pol.y,pol.x}$$

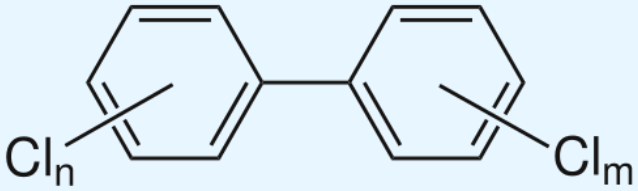
medium: e.g. water, air, lipid
pol.x: reference polymer
pol.y: test polymer

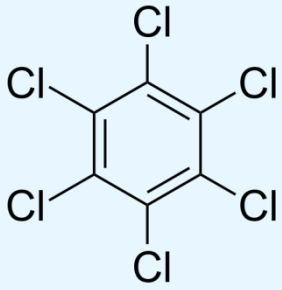
Polymers in passive sampling & dosing

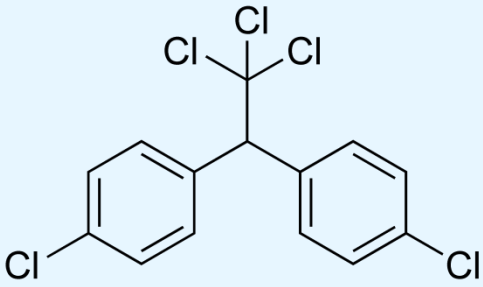
- **30-µm PDMS fiber** (Polymicro Techn.)
- **10-µm PDMS fiber** (Fiberguide Ind.)
- **AlteSil silicone sheet** (Altec)
- **SSP-M823** (Speciality Silicone Products)
- **BiscaSil PDMS coated fabric** (Biscor)
- **PDMS MDX4-4210** (Dow Corning)
- **PDMS DC1-2577** (Dow Corning)
- **silicone O-rings** (Altec)
- **silicone tubing**
- **hollow fibers**
- **silicone rods**
- **LDPE**

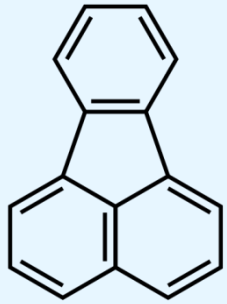
Chemicals in this study

- **25 PCBs + HCB**
- **HCHs (α, β, γ), o'p-DDT, p'p-DDT, DDEs, p'p-DDD, TNC**
- **10 PAHs in separate experiment**









Partitioning experiments

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  - **mass balance for confirmation**

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- $$K_{pol.x,pol.y} = \frac{C_{pol.x}}{C_{pol.y}}$$

High precision & accuracy of $K_{PDMS,PDMS}$

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  - **$K_{pol:fiber(PM)}$, $K_{pol:fiber(FG)}$!,**
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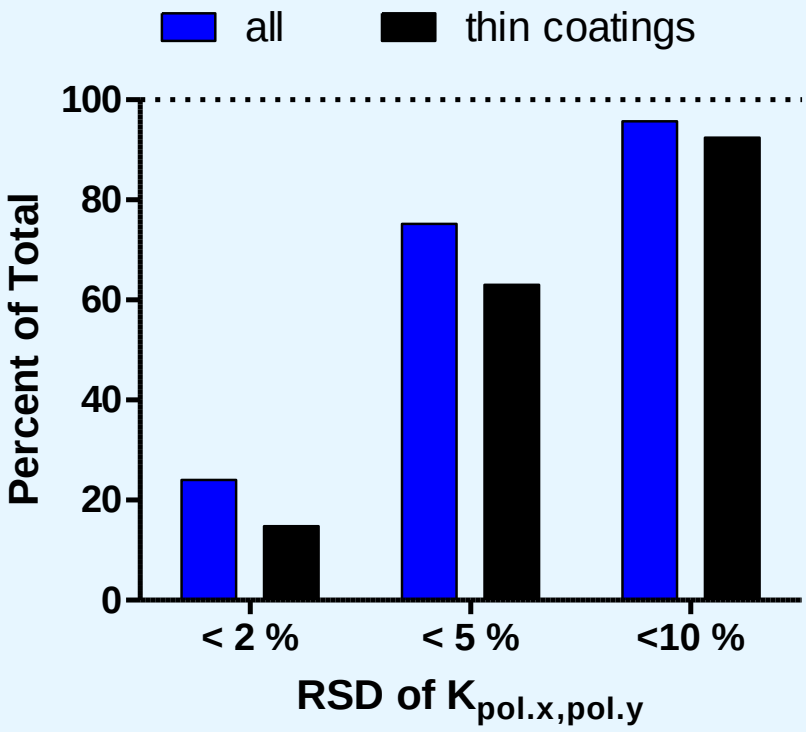

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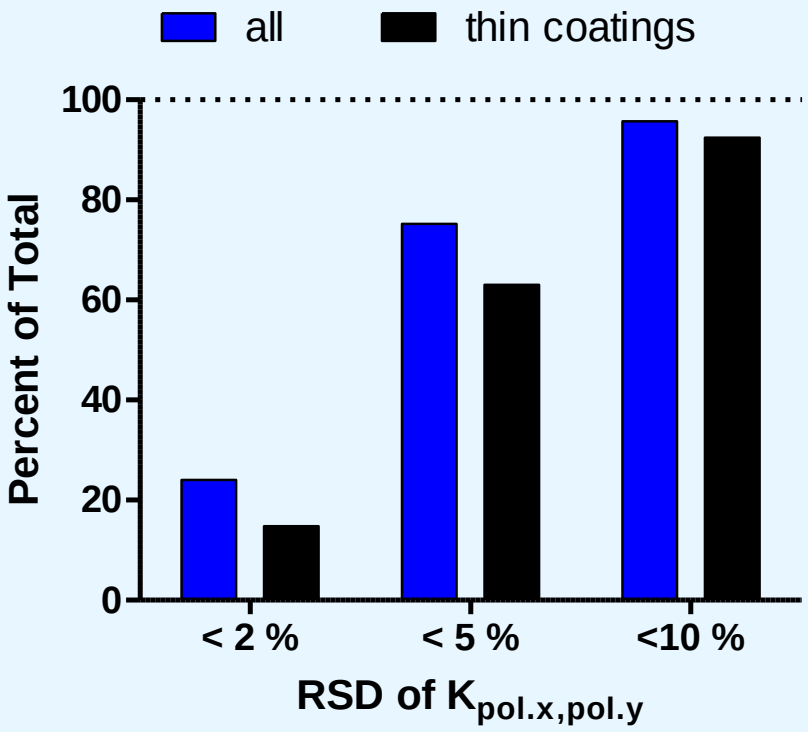
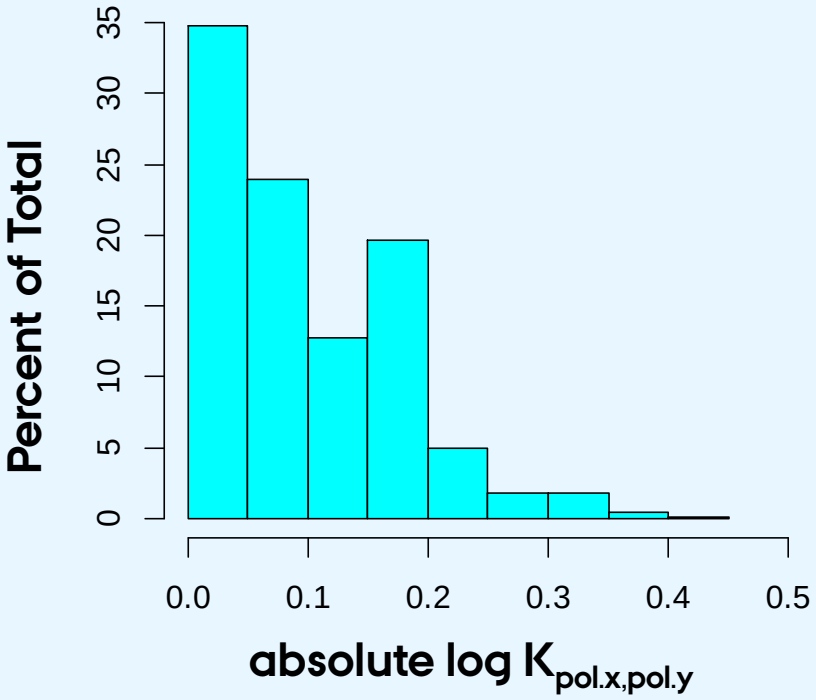
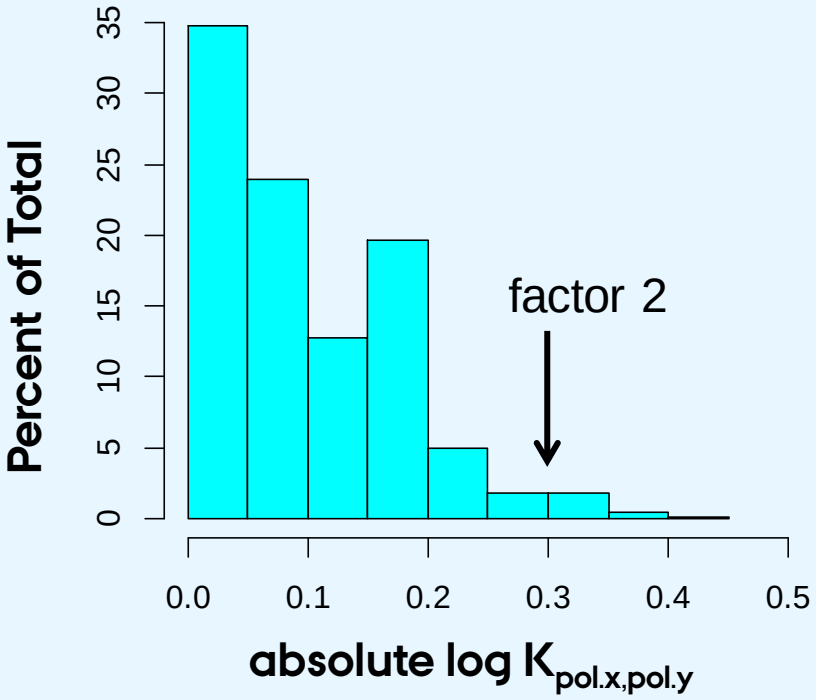
- **SE of $K_{pol.x,pol.y}$ ≤ log 0.005**



$K_{PDMS,PDMS}$


Percent of Total
0
5
10
15
20
25
30
35
0.0
0.1
0.2
0.3
0.4
0.5
absolute log K pol.x,pol.y

$K_{PDMS,PDMS}$



› **abs log $K_{pol.x,pol.y}$ < 0.3 98 %**

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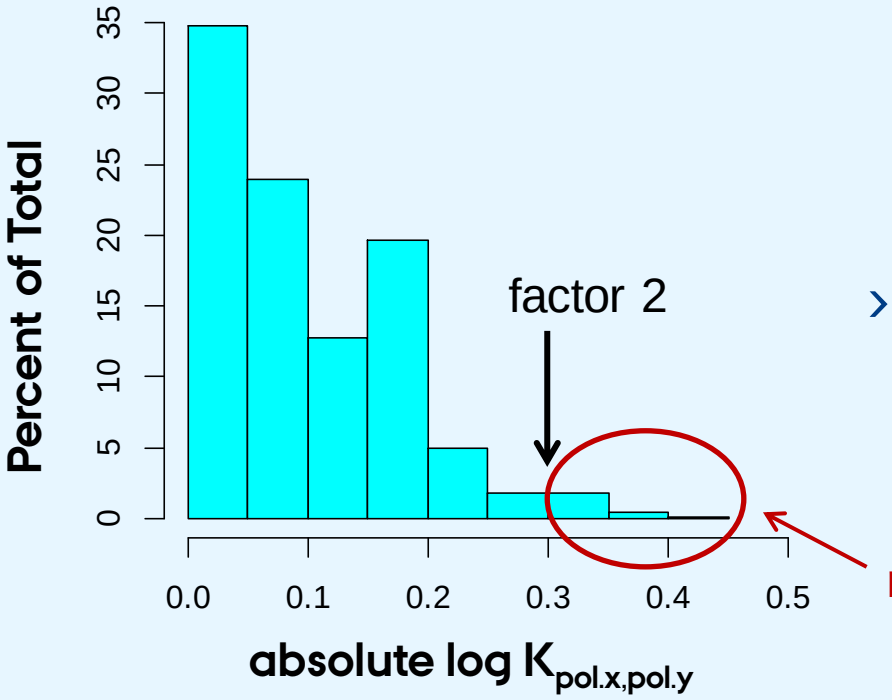

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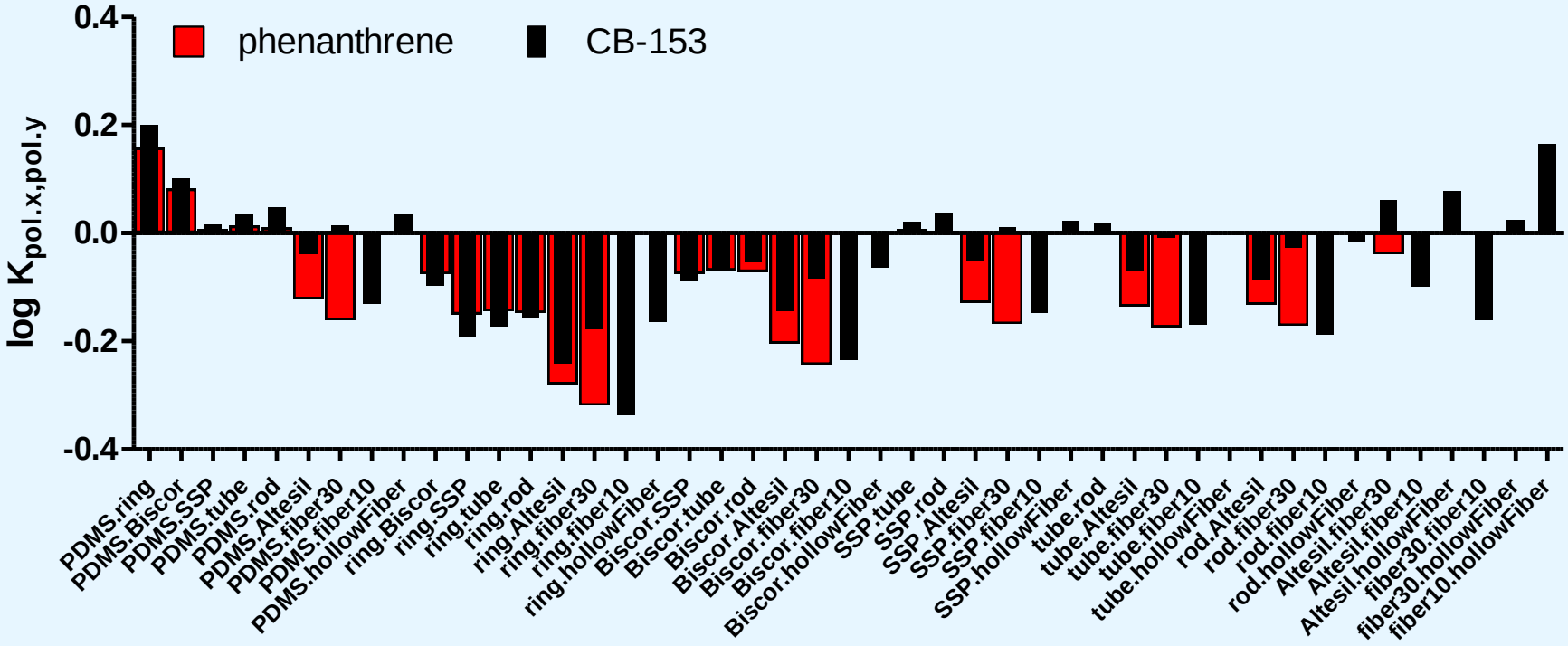
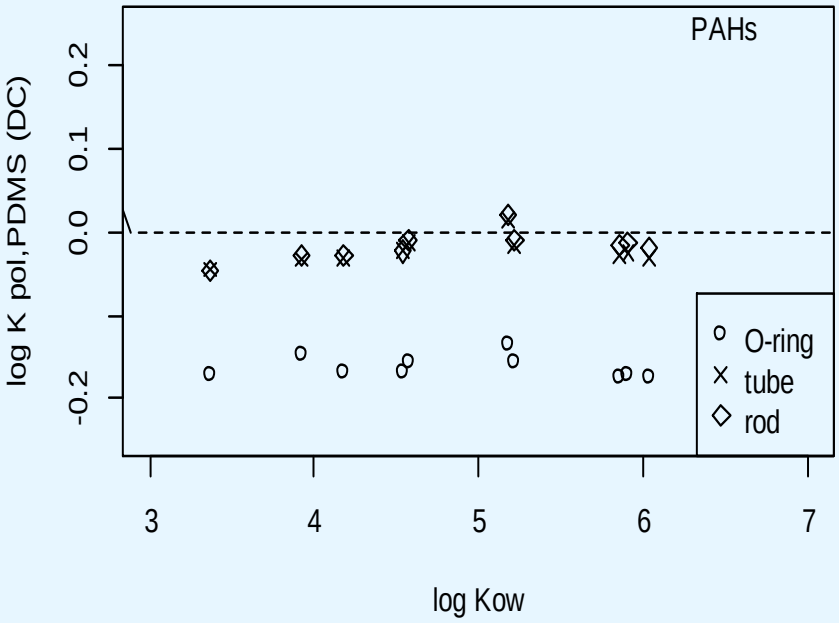
Example: phenanthrene & PCB153

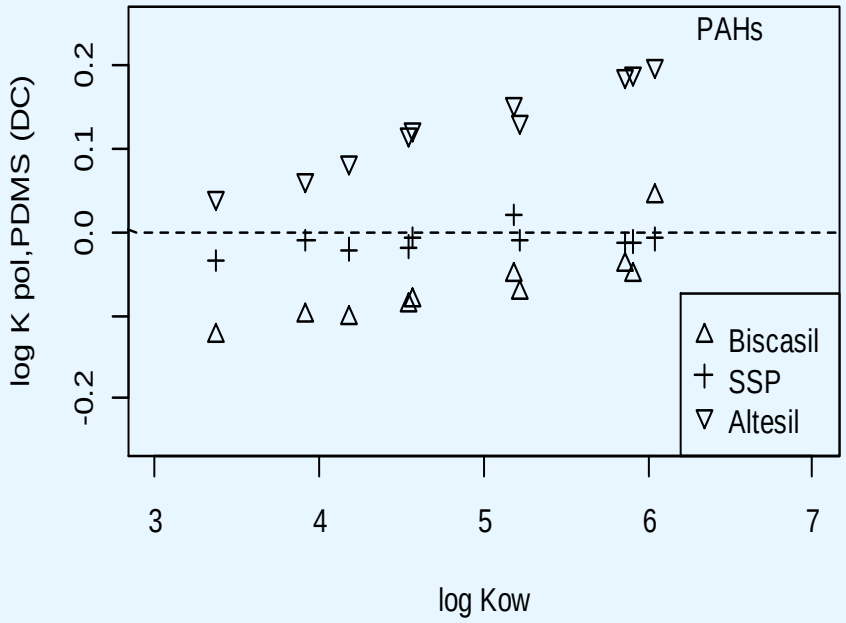


$K_{PDMS,PDMS} \neq 1$

- **different polymer** → substance-specific
- **fillers** → not substance-specific
- **uncertainty in $V_{polymer}$** → not substance specific

log $K_{pol.x,pol.y}$ – log K_{ow} relationship





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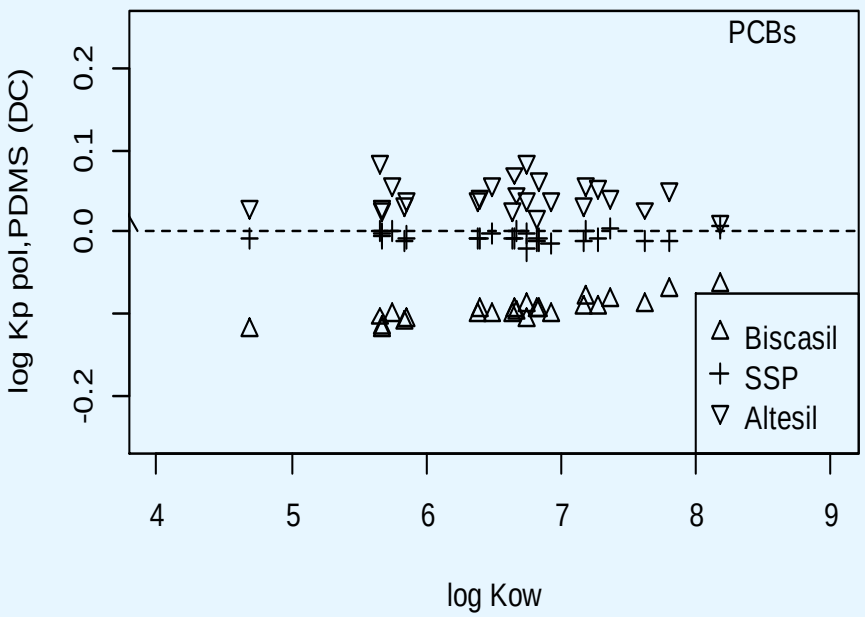
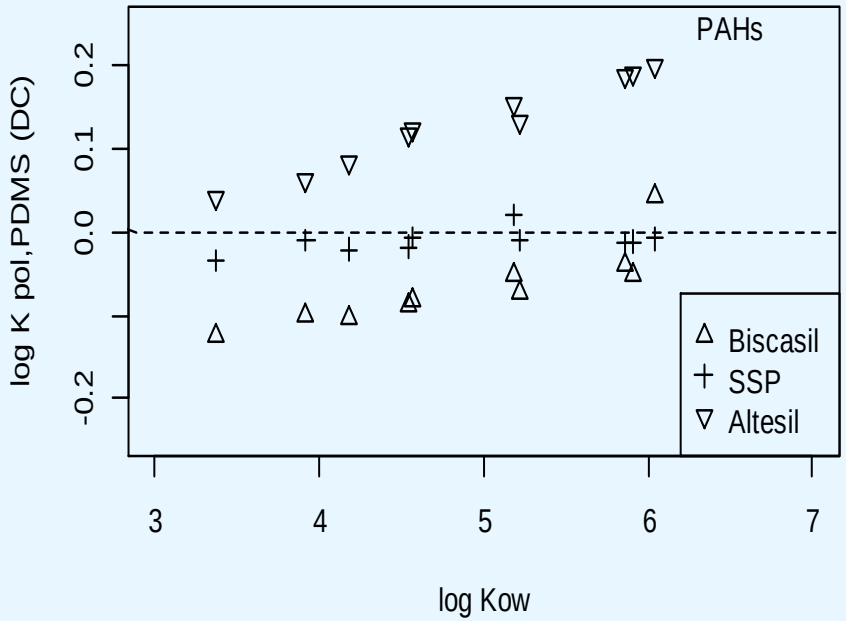
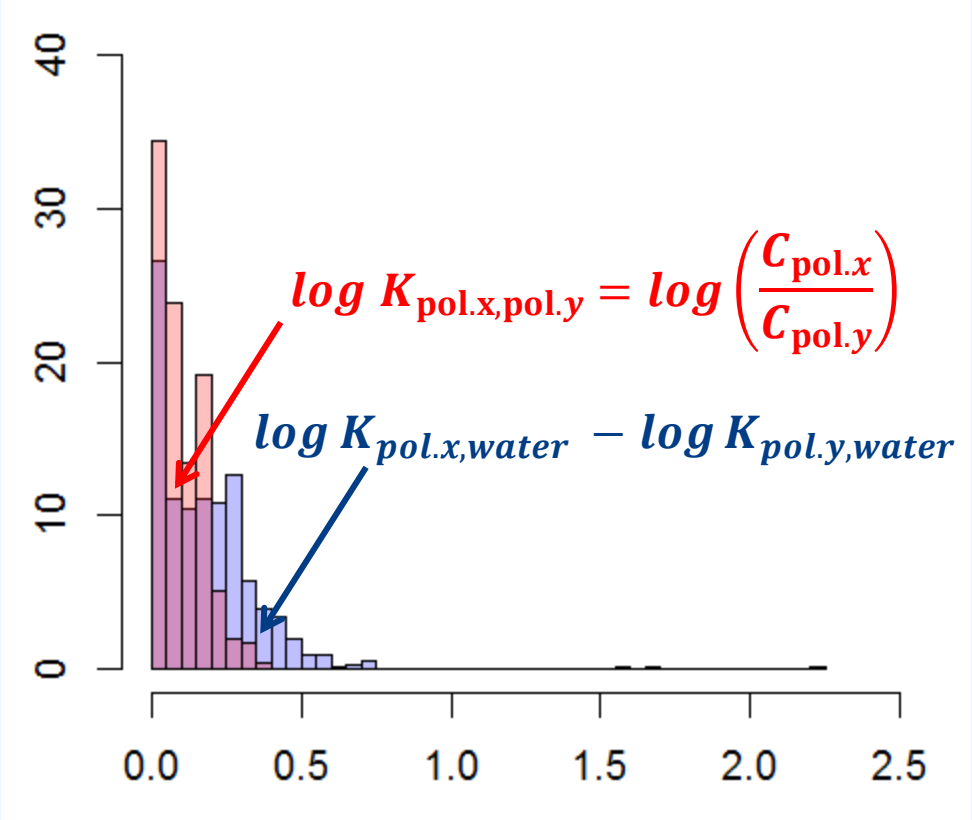




- **diatomic fillers in silicone O-rings**
- **higher affinities of some materials for more hydrophobic PAHs**

Relevance & implications



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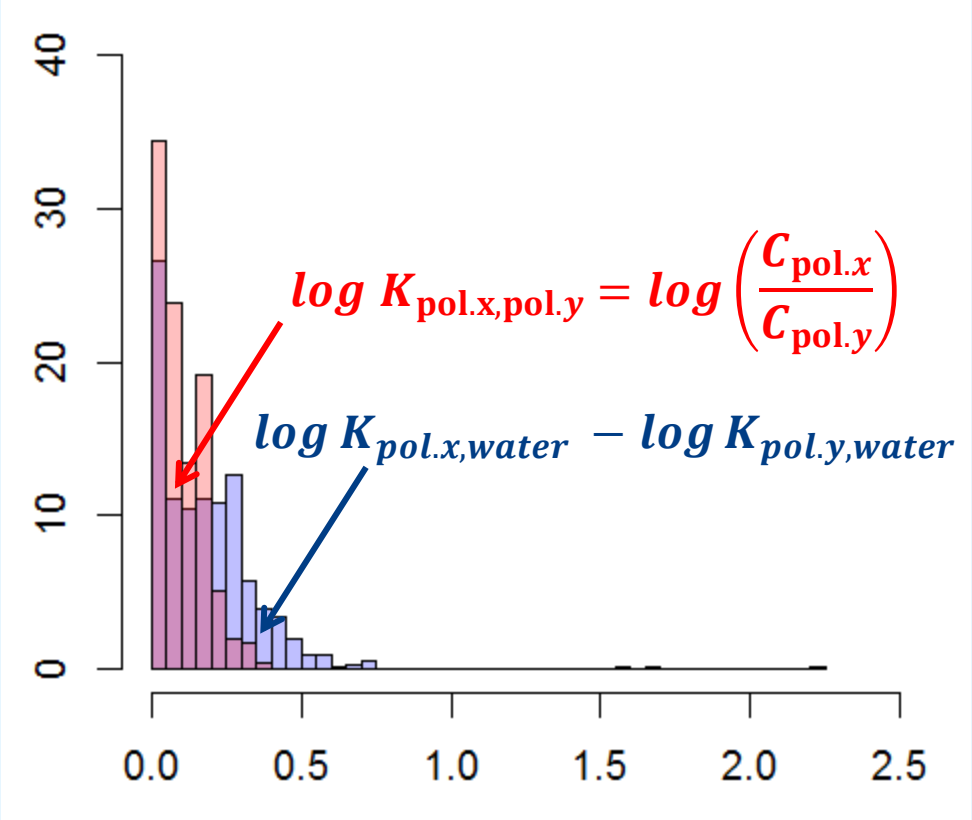

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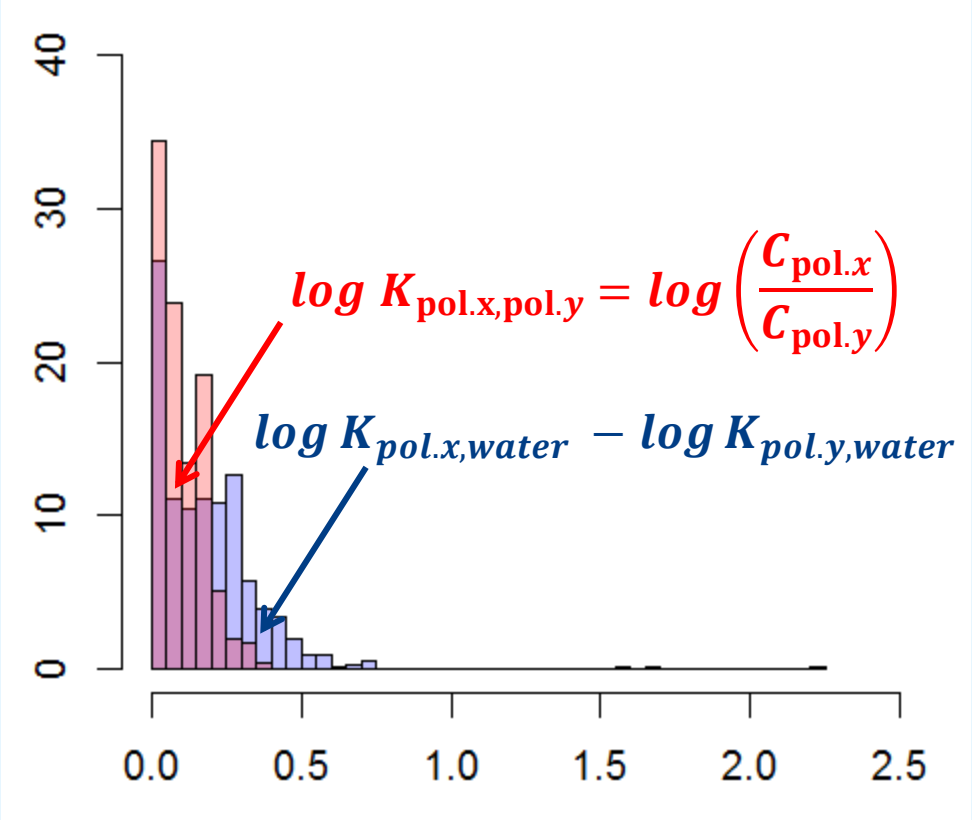

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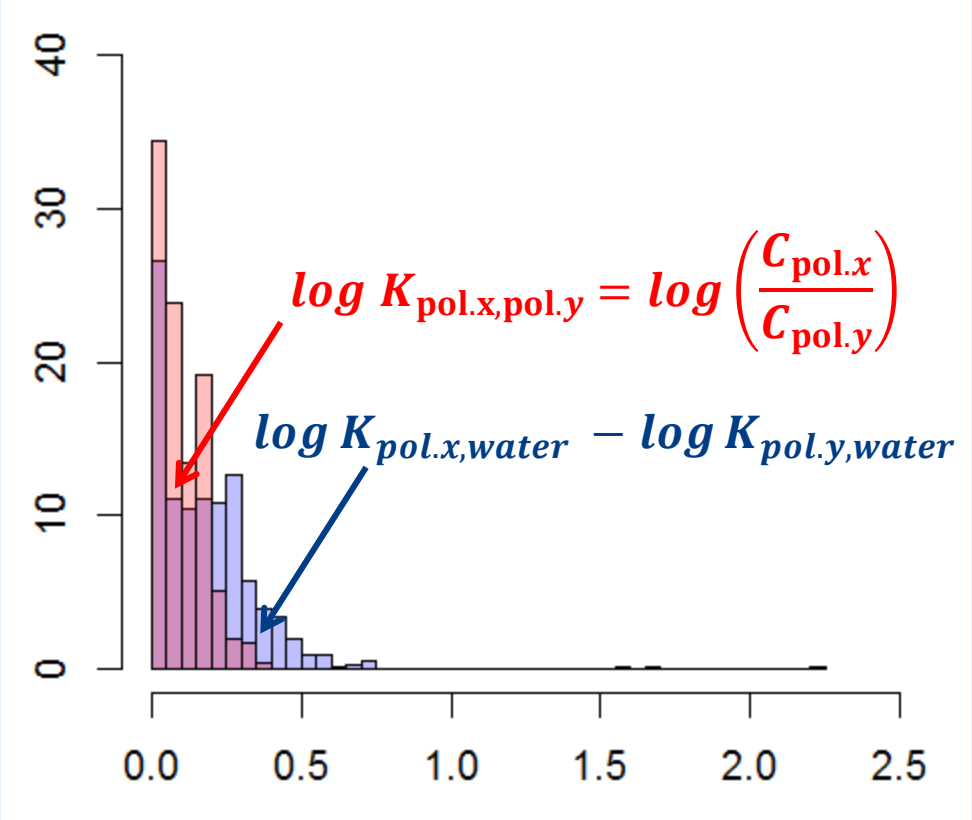

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- $K_{pol.x,pol.y}$ allows correction of existing $K_{polymer,water}$
- cross-consistency check now possible

Conclusions

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- **for PDMS $0.5 < K_{pol.x,pol.y} < 2$ (PAHs, PCBs, OCPs)**
- **little contribution of $K_{pol.x,pol.y}$ to uncertainty in $K_{polymer:water}$**

Thank you for your attention.

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