


Obstacles in Finding New POPs: Bioaccumulation and Toxicity

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Obstacles in Finding New POPs: Bioaccumulation and Toxicity

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Regulatory Efforts



STOCKHOLM CONVENTION

Persistence (P)	$t_{1/2} > 60$ days (water), $t_{1/2} > 180$ days (soil/sediment)
Bioaccumulation (B)	BCF/BAF $> 5'000$ L/kg ww, $\log K_{ow} > 5$
Toxicity (T)	human health or environmental hazard evidence
Long-Range Transport Potential (LRTP)	$t_{1/2} > 2$ days (air)
Assessment	POP

Regulatory Efforts



STOCKHOLM CONVENTION



Persistence (P)	$t_{1/2} > 60$ days (water), $t_{1/2} > 180$ days (soil/sediment)	$t_{1/2} > 40 - 60$ days (water), $t_{1/2} > 120 - 180$ days (soil/sediment); vP $t_{1/2} > 60$ days (water), $t_{1/2} > 180$ days (soil/sediment)
Bioaccumulation (B)	$BCF/BAF > 5'000$ L/kg ww, $\log K_{ow} > 5$	$BCF > 2'000$ L/kg ww; vB $BCF > 5'000$ L/kg ww
Toxicity (T)	human health or environmental hazard evidence	$NOEC/EC_{10} < 0.01$ mg/L (marine or freshwater organisms), other classification (CMR, STOT RE)
Long-Range Transport Potential (LRTP)	$t_{1/2} > 2$ days (air)	-
Assessment	POP	PBT/vPvB

Choosing A POP Candidate

Initial screening

	LogK _{ow}	P	B	T	LRTP
#1	6.27	Exp. + Est.	Exp. + Est.	Exp. + Est.	Est.
#2	6.91	Exp. + Est.	Exp. + Est.	Exp. + Est.	Est.
#3	7.25	Exp. + Est.	Exp. + Est.	Exp. + Est.	Est.
#4	6.31	Est.	Exp. + Est.	Exp. + Est.	Est.
#5	11.46	Exp. + Est.	Est.	Exp. + Est.	Est.
#6	11.27	Exp. + Est.	Exp. + Est.	Exp. + Est.	Est.
#7	13.64	Exp. + Est.	Exp. + Est.	Exp. + Est.	Est.
#8	11.95	Exp. + Est.	Exp. + Est.	Exp. + Est.	Est.
#9	7.37	Exp. + Est.	Est.	Exp. + Est.	Est.

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	LogK _{ow}	P	B	T	L RTP
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B and T assessment based on

- Experimental data: not reliable, inadequate testing guidelines (TGs)
- Estimated data

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31 experimental results

B 6 studies using OECD TG 305, 14 in total

T 2 studies using OECD TG 203, 17 in total

B and T assessment based on

- Experimental data: not reliable, inadequate testing guidelines (TGs)
- Estimated data

Experimental Testing B and T

Main limitations when $\log K_{ow}$ is very high

Solubility

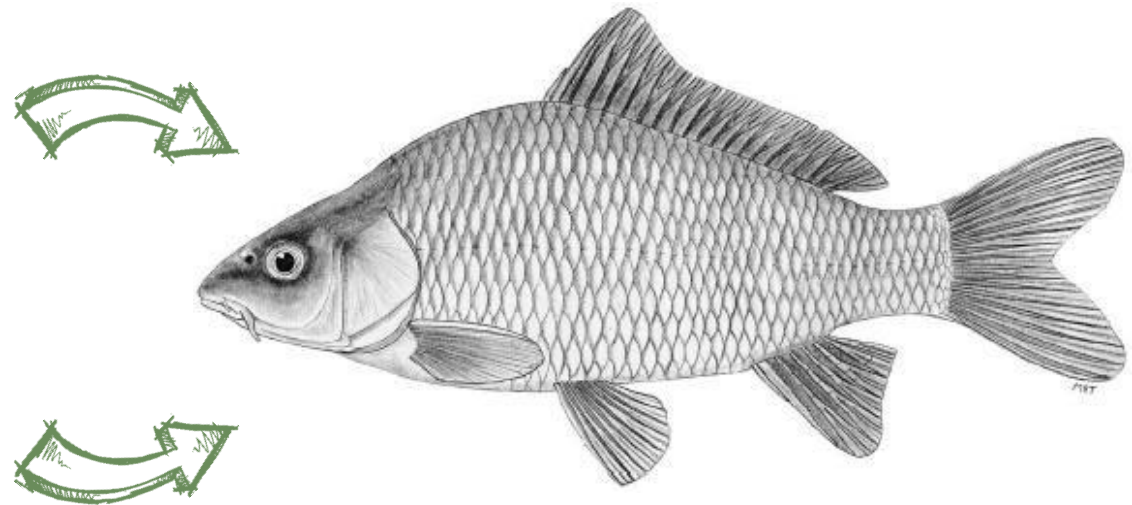
Thermodynamics

Small solubilized fraction

Timescale

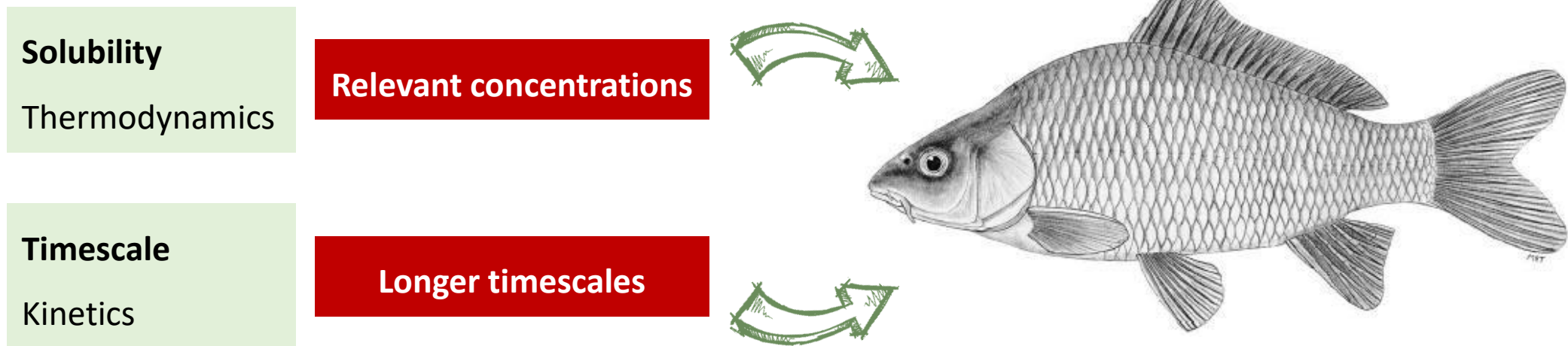
Kinetics

Slow respiratory uptake



Experimental Testing B and T

Main limitations when $\log K_{ow}$ is very high



Bioaccumulation Concepts

BCF	Bioconcentration factor	$C_{\text{org}}/C_{\text{W}}$
BAF	Bioaccumulation factor	$C_{\text{org}}/C_{\text{W}}$
BMF	Biomagnification factor	$C_{\text{pred}}/C_{\text{prey}}$
TMF	Trophic magnification factor	10^m

Experimental Guidelines

Aquatic bioaccumulation testing

OECD TG 305 Bioaccumulation in Fish: Aqueous and Dietary Exposure (2012)

OECD TG 305 Bioconcentration: Flow-through Fish Test (1996)

OECD TG 305C Bioaccumulation: Test for the Degree of Bioconcentration in Fish (1981)

OECD TG 305D Bioaccumulation: Static Fish Test (1981)

Dietary bioaccumulation for low solubility substances ($\log K_{ow} > 5$)

- Generates BMF
- 60 days exposure
- May involve passive dosing systems

Experimental Guidelines

Aquatic acute toxicity testing

OECD TG 203 Fish, Acute Toxicity Test (1992)



Limited recommendations for hydrophobic substances

- Static, semi-static, flow-through setups
- When necessary, use of organic solvents, emulsifiers, or dispersants
- No dietary exposure, passive dosing

Experimental Guidelines

Aquatic acute toxicity testing

OECD TG 203 Fish, Acute Toxicity Test (1992)



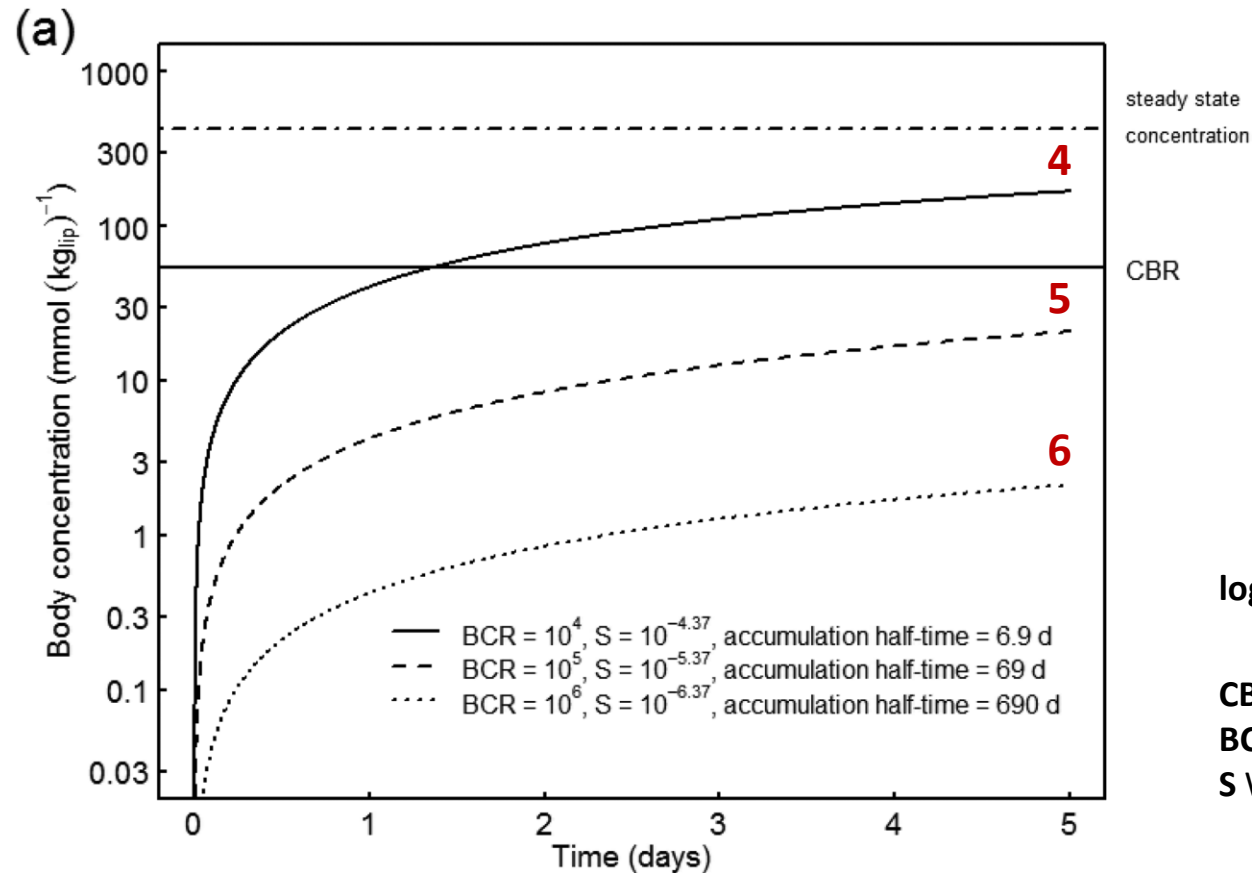
Limited recommendations for hydrophobic substances

- Static, semi-static, flow-through setups
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- No dietary exposure, passive dosing

**Acute aquatic toxicity testing
for very high hydrophobicity
substances?**

Toxicity

High hydrophobicity compounds



$$\log \text{BCR} \approx \log K_{ow}$$

CBR Critical Body Residue
BCR Bioconcentration Ratio
S Water Solubility

REACH Registration Dossiers

Aquatic bioaccumulation and acute toxicity

- #3** In a 96-h acute toxicity study, zebra-fish (*Brachydanio rerio*) were exposed to test item at nominal concentrations of 0 (control, solvent control) and 100 mg/L under static conditions. The 96-h LC50 was > 100 mg/L. No sublethal effects were observed and no mortalities were observed in the blank and solvent control.
- Effect concentrations exceeding solubility of substance in test medium: yes
- #5** Although this study was performed above water solubility level, under the study conditions no toxicity to the organisms was detected and no visible effects occurred during the 96-hour test period.
- #6** The 4-day dynamic toxicity of #6 was determined in bluegill fingerlings at nominal concentrations up to 100 ppm. No mortality and no effect on behaviour were observed, but the concentrations were not analytically verified, and visible precipitations accumulated at the bottom of the tanks. Due to the low water solubility of the test substance, the result is not conclusive.

❌❌❌ 3 of the REACH registered compounds were registered after 2012 ❌❌❌
OECD TG 305 (Dietary Exposure) is not used in any of these registrations

Conclusions

Call for updated testing guidelines and regulation

1. OECD TGs Update

- OECD TG 203 (acute aquatic T): no clear strategy for low solubility chemicals, e.g., passive dosing systems, dietary exposure
- Should acute aquatic T still be measured for high K_{ow} chemicals?

2. Routine use of standardized guidelines

- POP nomination and/or registration dossiers should not accept unreliable experimental data using outdated or inadequate testing guidelines, e.g., “testing above water solubility”

3. Stockholm Convention and REACH

- BMF and TMF: include parameters in the decision algorithm, clarify thresholds
- More adequate T requirements, e.g., according to physico-chemical properties not tonnage band

Acknowledgements

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Questions?

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Thank you!