



Bioconcentration of cationic surfactants in rainbow trout

Michael S. McLachlan¹, Amelie Kierkegaard¹, Michael Strandell¹, Bo Yuan¹,
Chang'er Chen¹, James Armitage², Jon Arnot³, Steven Droge⁴

¹Department of Environmental Science and Analytical Chemistry, Stockholm University

²AES Armitage Environmental Sciences, Inc.

³ARC Arnot Research and Consulting

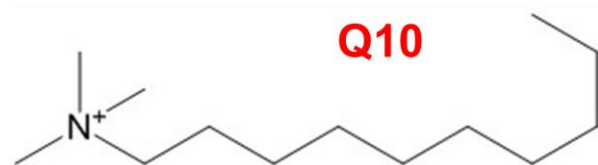
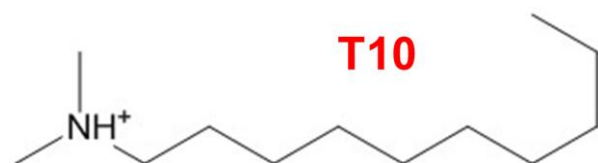
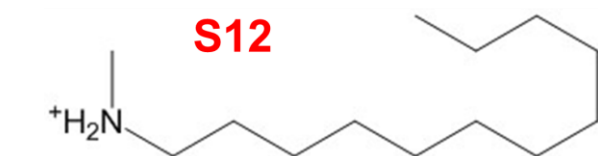
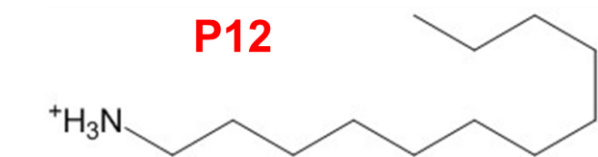
⁴Institute for Biodiversity and Ecosystem Dynamics (IBED), University of Amsterdam

Presentation at the 40th Annual Meeting of SETAC North America, Toronto, 3-7 Nov 2019

Background

- Cationic surfactants are an important class of chemicals released to the environment
- Sorb strongly to membranes, increasing likelihood of strong bioaccumulation
- Sorb strongly to many other surfaces too, making BCF measurements difficult
- Dearth of BCF measurements
- Measured here for model evaluation

Test chemicals: alkyl amines and quaternary ammonium cations



MIX 1

P9	T10	P12	T13	Q14	P16
----	-----	-----	-----	-----	-----

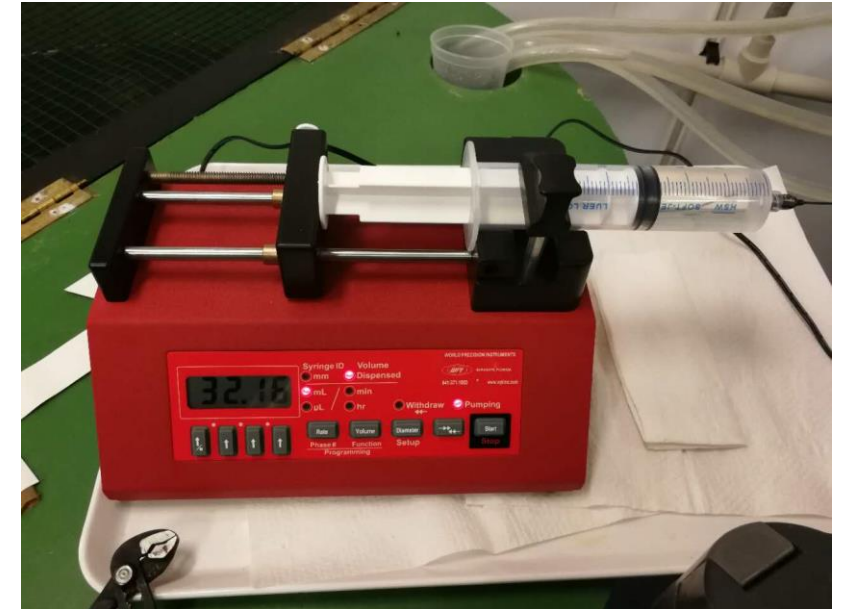
MIX 2

T9	Q10	S12	P13	T14	S16
----	-----	-----	-----	-----	-----

BCF experiment, environmental conditions

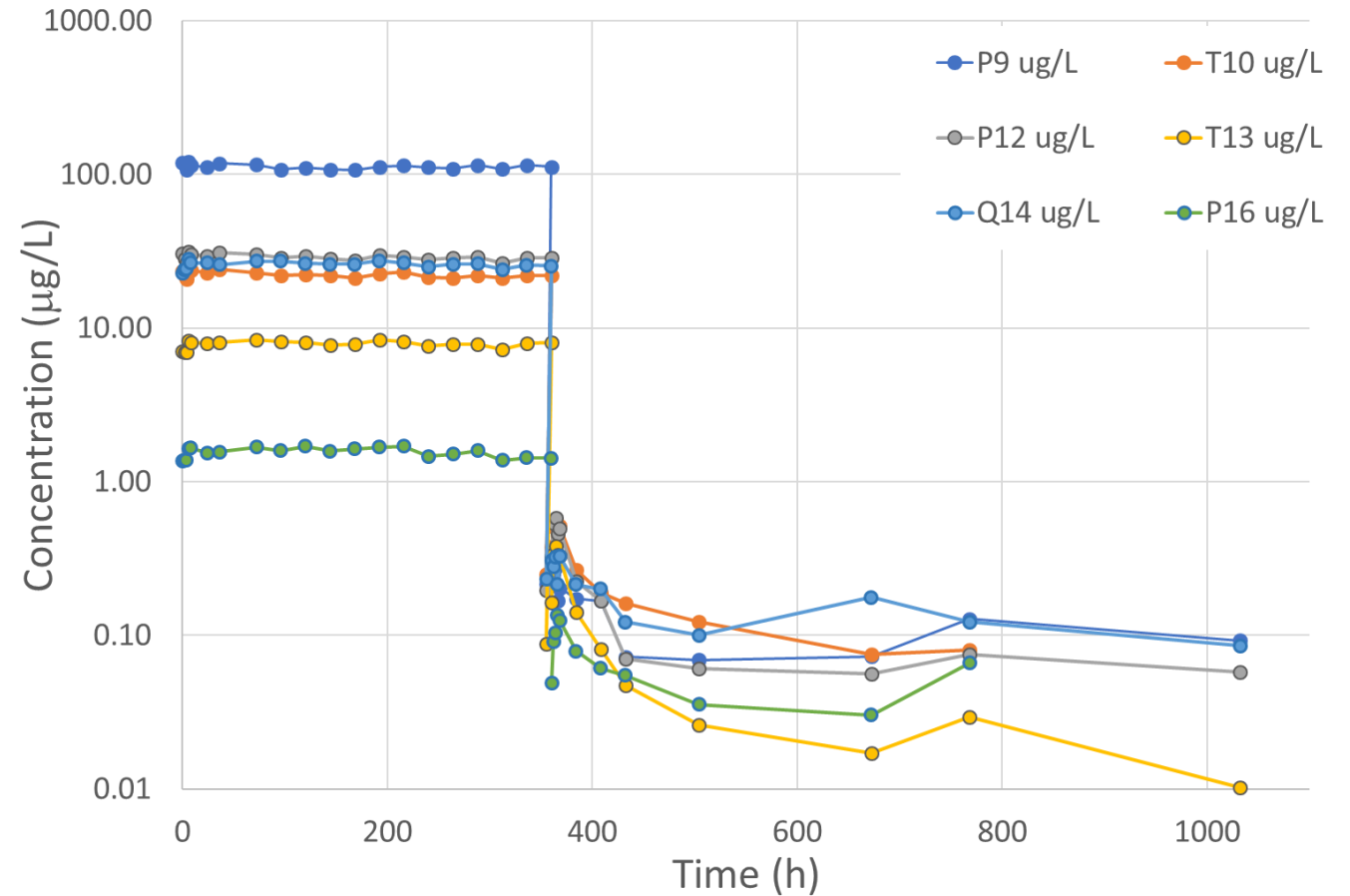


- Flow-through fiberglass aquaria
- Water residence time 4 h
- Water filters changed daily
- Feces siphoned off daily (kept TOC to $\sim 5 \text{ mg C L}^{-1}$)
- Test chemicals delivered in methanol with syringe pump



MIX1 pH: Concentrations in Water

- Water sampled directly into autosampler vial
- Analysis by direct injection



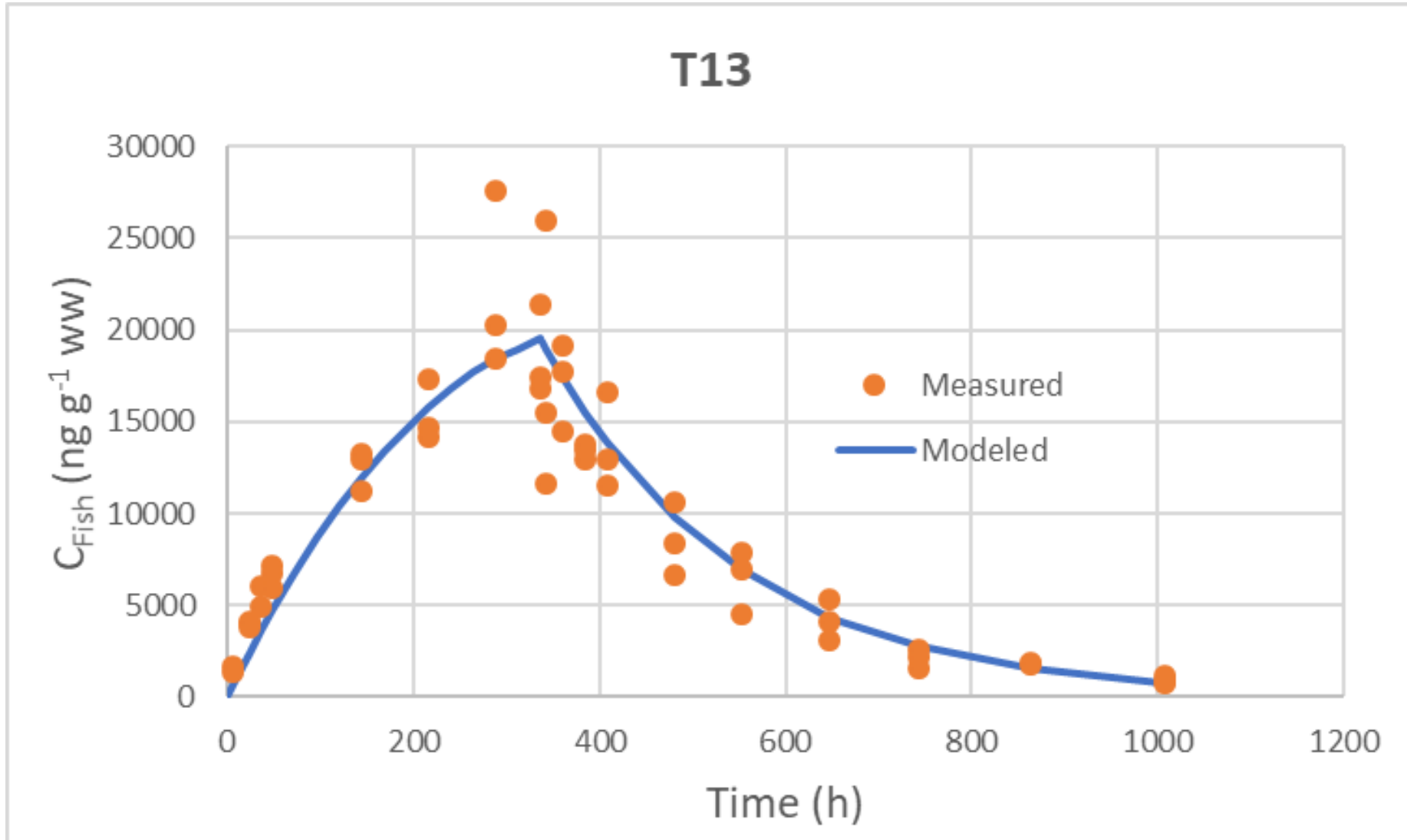
Fish exposure



- 3 experiments:
 - a) MIX 1, pH 7.8
 - b) MIX 2, pH 7.8
 - c) MIX 1, pH 6.3
- Exposure phase 14 d, 8 sampling points
- Depuration phase 28 d, 10-12 sampling points
- 3 fish per sampling point
- Juvenile rainbow trout
- Feeding 1% of body weight per day

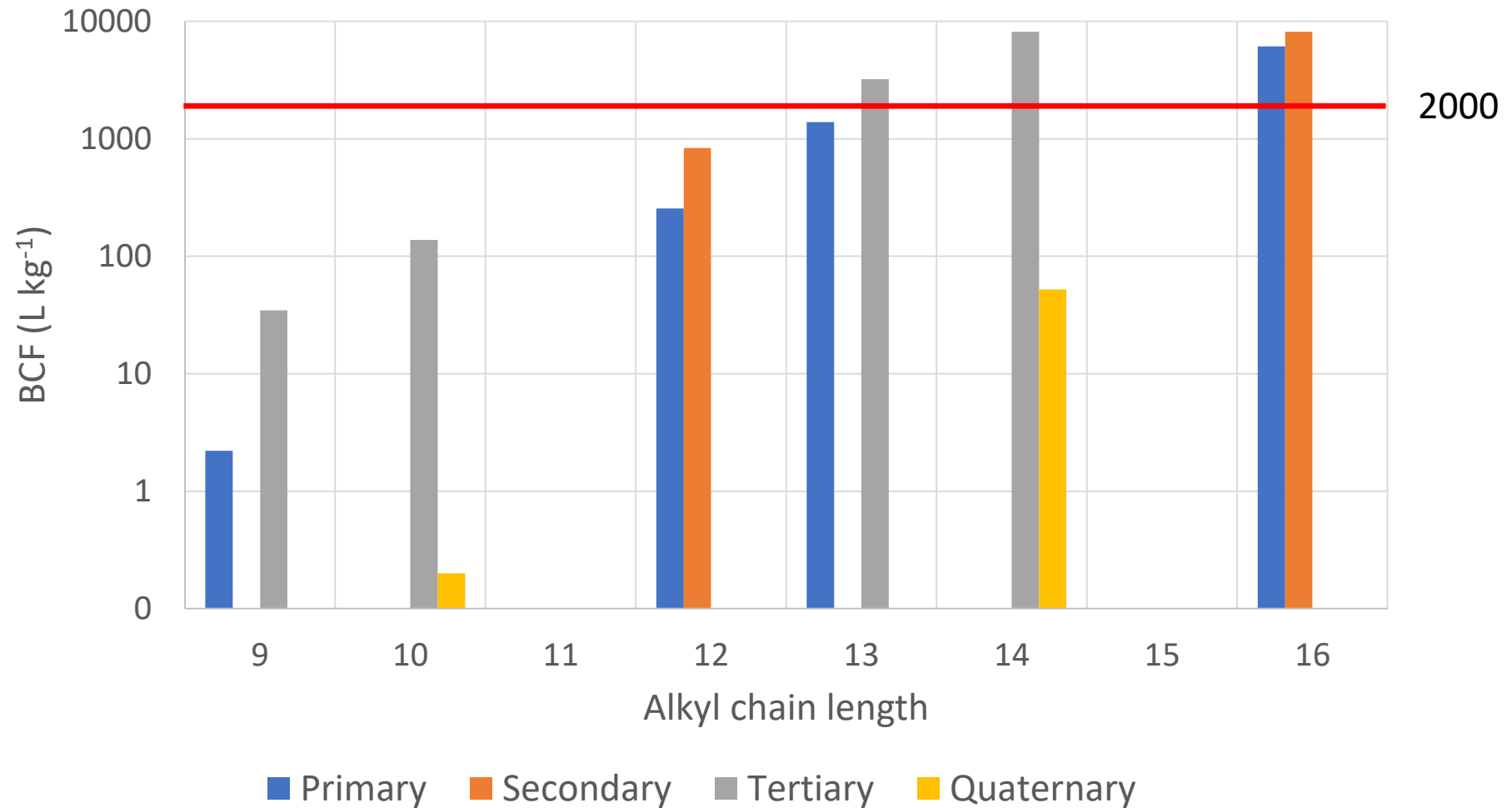
Kinetics in fish

(1 compartment model)

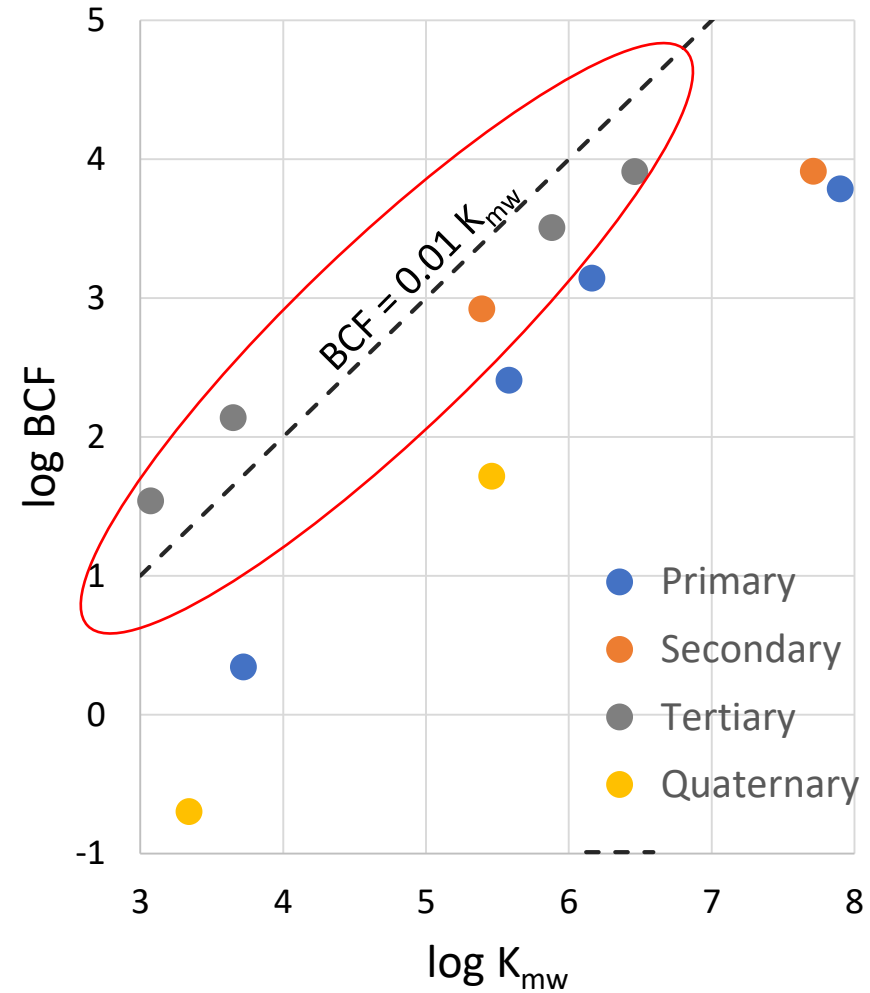


BCF

(pH = 7.8)

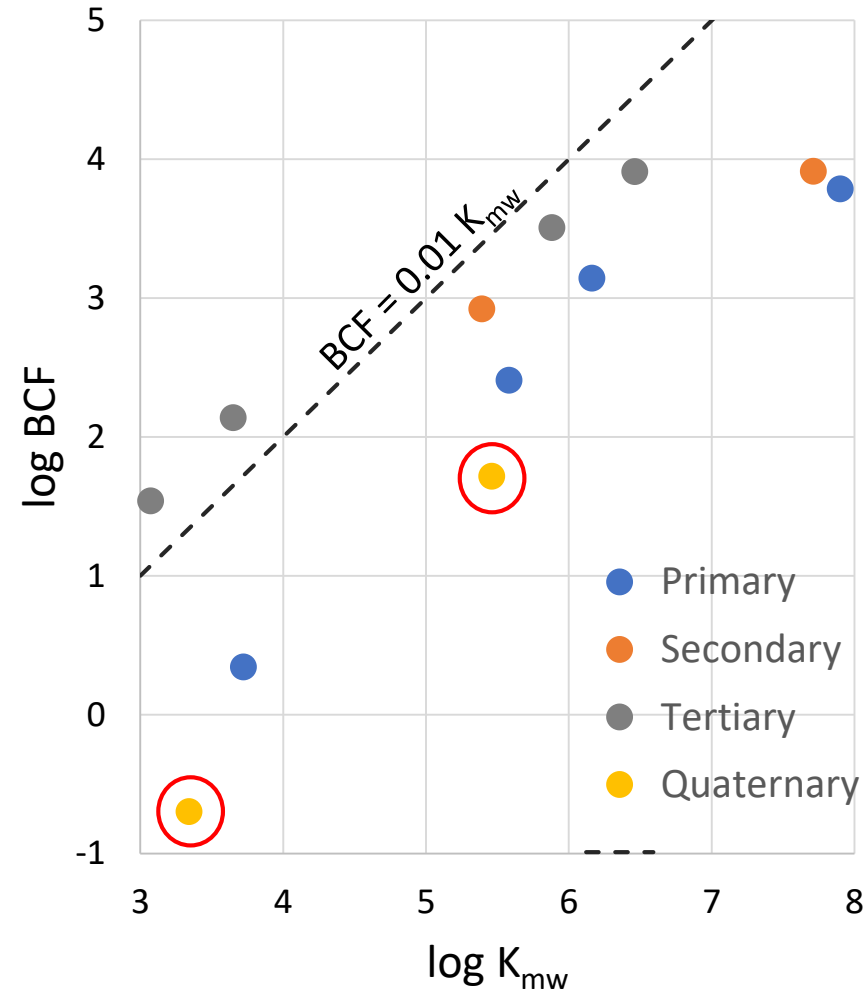


BCF membrane-water partition coefficient K_{mw}



Secondary and tertiary amines
- Equilibrium partitioning to membranes?

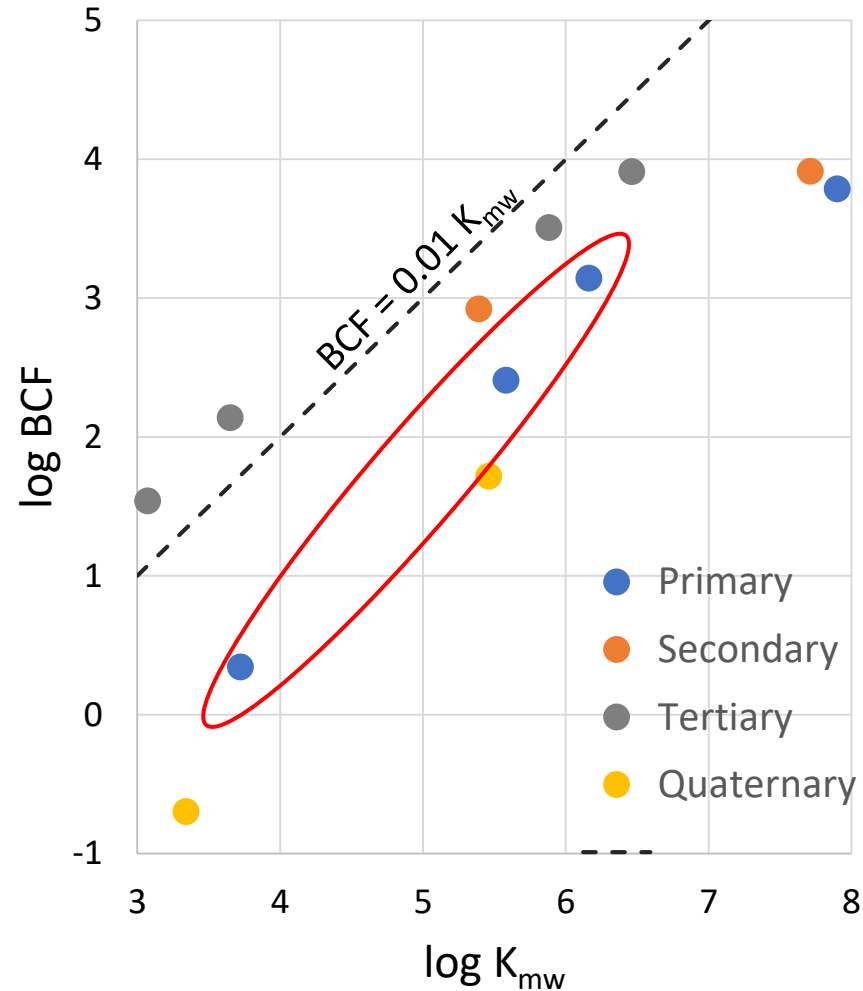
BCF membrane-water partition coefficient K_{mw}



Secondary and tertiary amines
- Equilibrium partitioning to membranes?

Quaternary amines
- Minimal systemic uptake.
- Surface sorption dominated.

BCF membrane-water partition coefficient K_{mw}

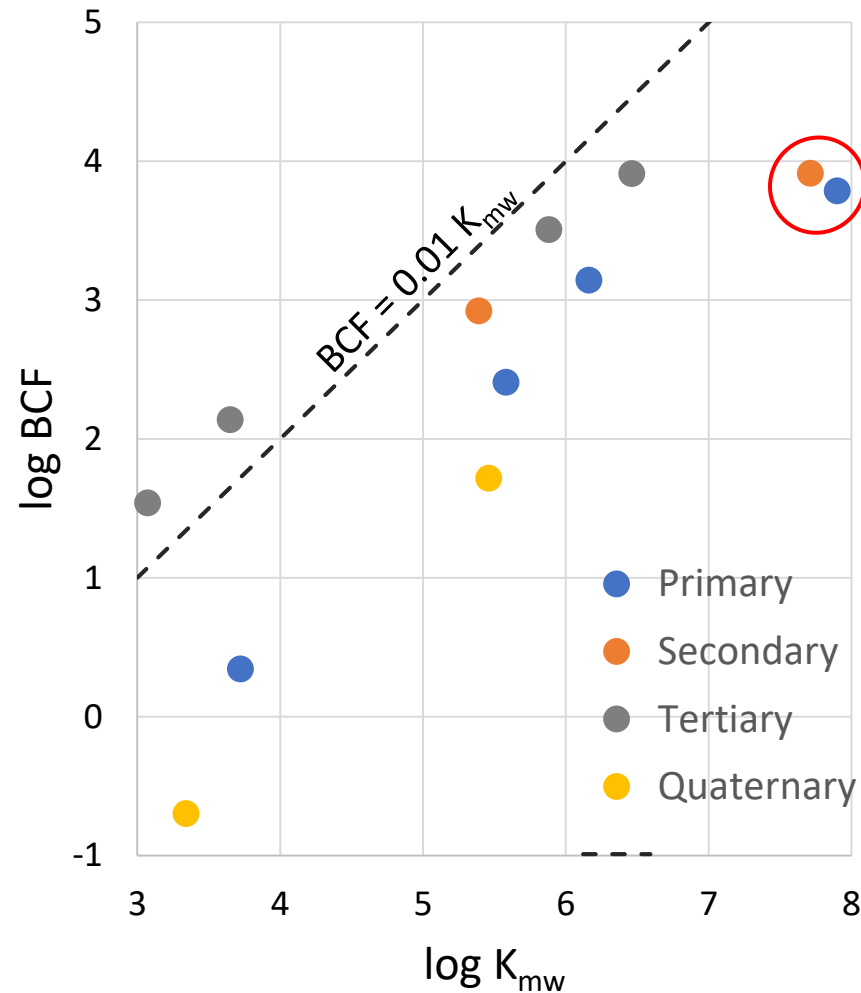


Secondary and tertiary amines
- Equilibrium partitioning to membranes?

Quaternary amines
- Minimal systemic uptake.
- Surface sorption dominated.

Primary amines
- High inter-individual variability.
- Metabolism?

BCF membrane-water partition coefficient K_{mw}



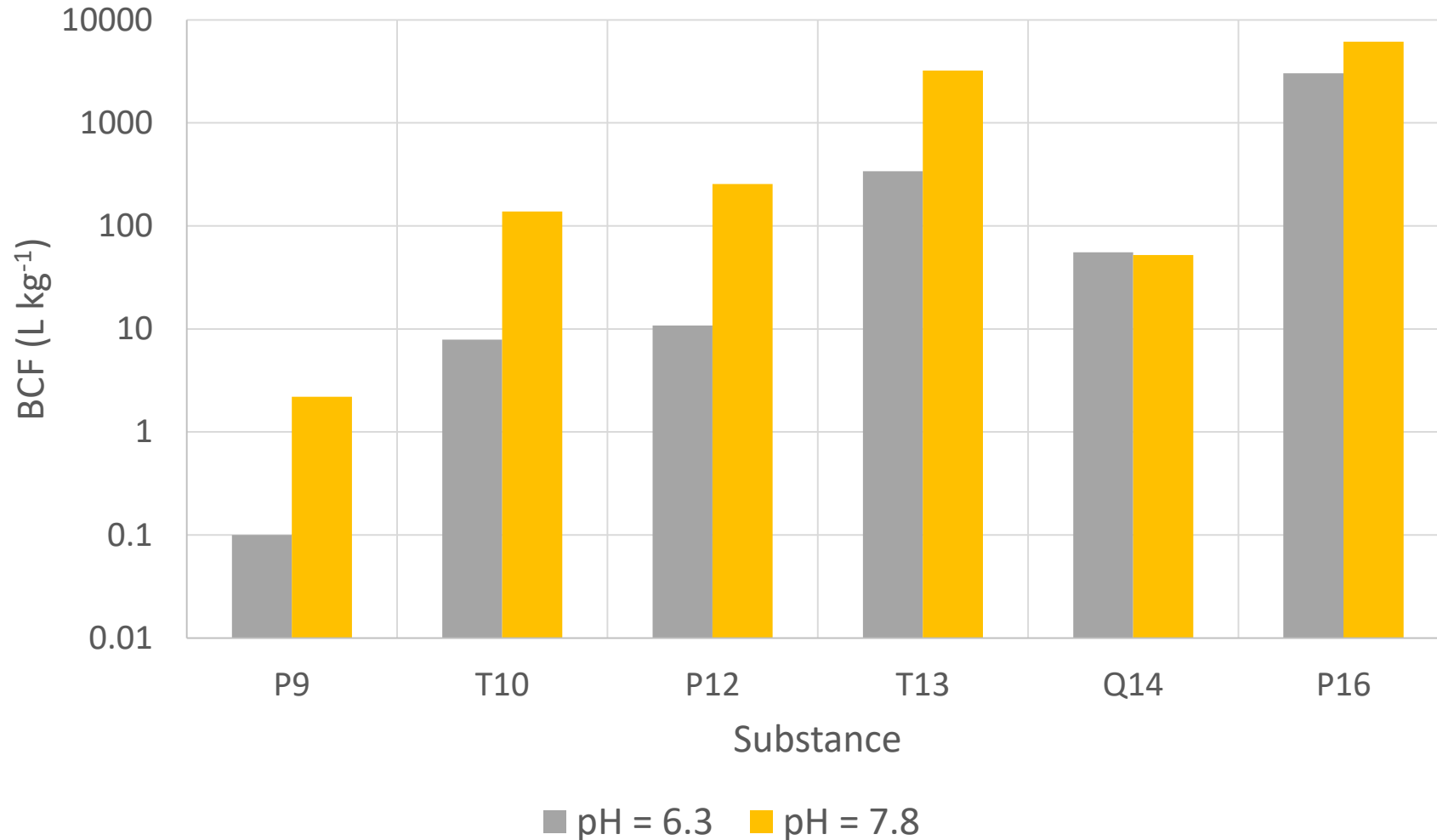
Secondary and tertiary amines
- Equilibrium partitioning to membranes?

Quaternary amines
- Minimal systemic uptake.
- Surface sorption dominated.

Primary amines
- High inter-individual variability.
- Metabolism?

Long-chained amines
- ?

BCF as a function of pH



Secondary and tertiary amines

- (*Equilibrium partitioning to membranes?*)
- Only neutral form bioavailable.

Quaternary amines

- Minimal systemic uptake.
- Surface sorption dominated.



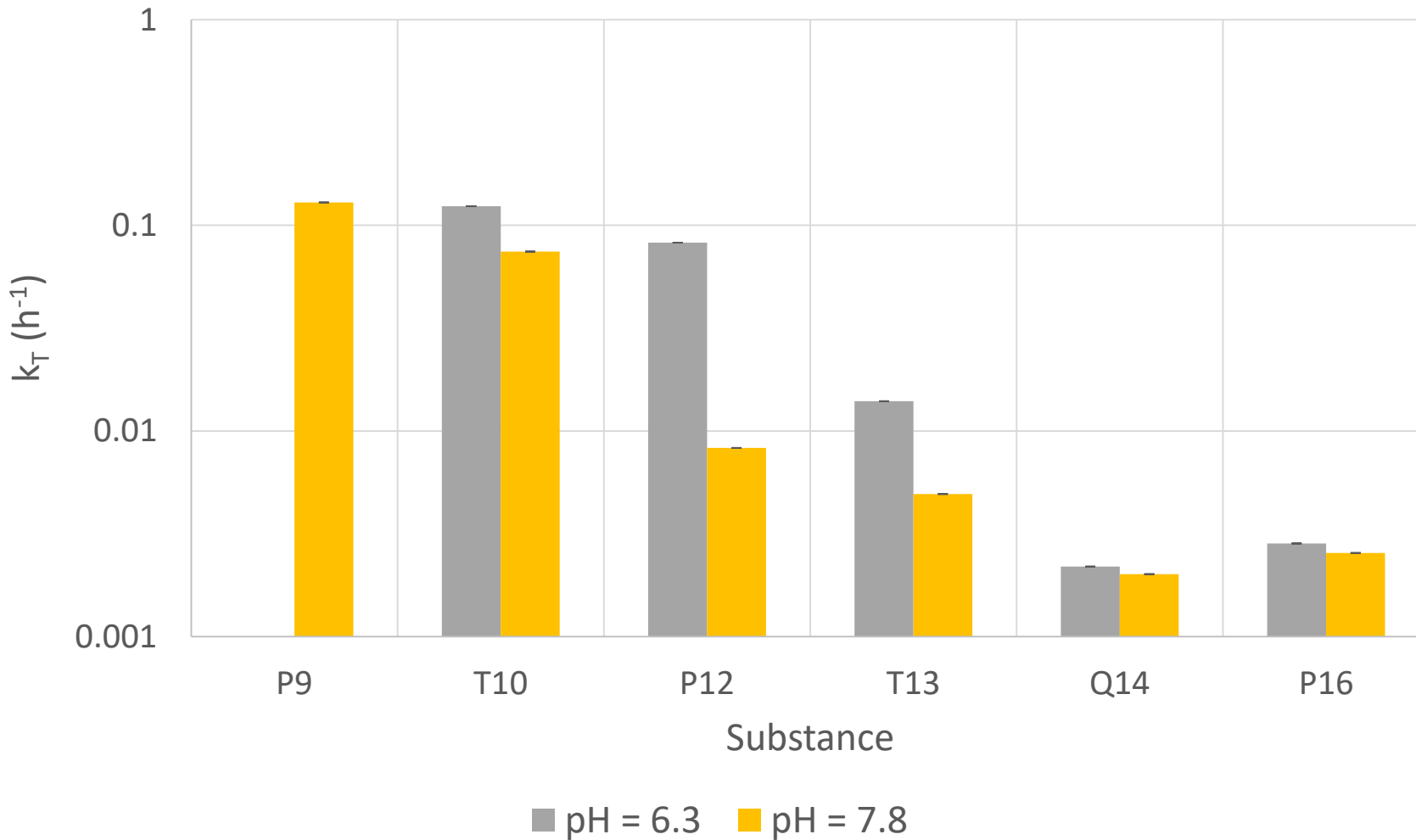
Primary amines

- High inter-individual variability.
- Metabolism?

Long-chained amines

- ?

k_T as a function of pH



Secondary and tertiary amines

- (*Equilibrium partitioning to membranes?*)
- Only neutral form bioavailable.
- Metabolism plays minor role.

Quaternary amines

- Minimal systemic uptake.
- Surface sorption dominated.



Primary amines

- High inter-individual variability.
- ~~Metabolism?~~

Long-chained amines

- Metabolism!?

Conclusion

We haven't figured it out yet....

So on to modeling with BIONIC!!

Secondary and tertiary amines

- (*Equilibrium partitioning to membranes?*)
- Only neutral form bioavailable.
- Metabolism plays minor role.

Quaternary amines

- Minimal systemic uptake.
- Surface sorption dominated.



Primary amines

- High inter-individual variability.
- Metabolism?

Long-chained amines

- Metabolism!?

Summary

- BCF of alkylamines increases with chain length and B threshold is exceeded for some
- BCF of amines is pH dependent, suggesting that uptake of the neutral species dominates
- Elimination of some amines is also pH dependent, suggesting that it is not dominated by metabolism (at least at the lower pH)
- BCF of quaternary ammonium compounds low, independent of pH

Acknowledgements

- Cefic LRI for funding (ECO37)
- Gisela Horlitz for assisting with the experiments