Supporting information

Predicting Sediment Sorption Coefficients for Linear Alkylbenzene Sulfonate Congeners from Polyacrylate-Water Partition Coefficients at Different Salinities

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Table S1. Ion Composition of the Artificial GP2 Seawater (SW) and Dutch Standard Water (DSW).

	SW	DSW
	mmol L^{-1}	mmol L^{-1}
Na^{+} *	418	11
Mg^{2+}	46.73	0.30
Ca^{2+}	8.98	1.36
K^{+}	8.92	0.20
Sr^{2+}	0.08	
Cl^{-}	480	2.70
SO_4^{2-}	24.80	0.30
HCO_3^{-}	2.02	1.40
Br^{-}	0.74	
$B_4O_7^{2-}$	0.09	

*10 mM NaN_3 is considered for the calculation of Na^{+} content in SW and DSW solutions.

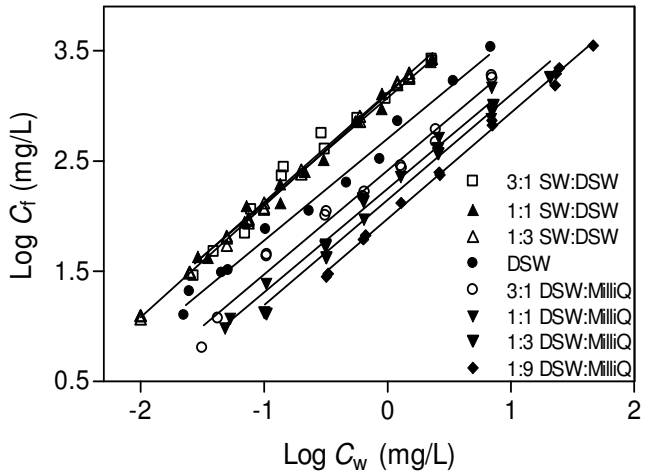

Figure S1. Fiber-water isotherms for C_{12}-2-LAS at different seawater and freshwater dilutions.

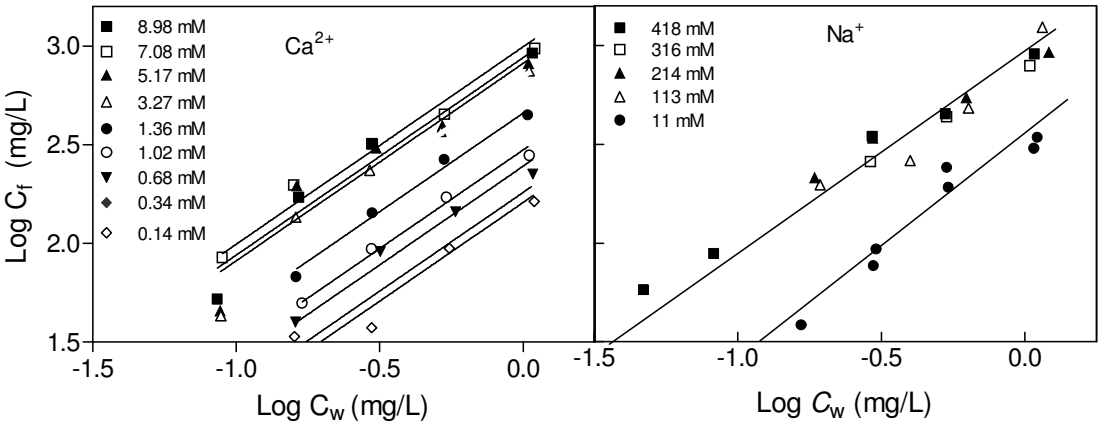

Figure S2. Fiber-water isotherms for C_{12}-2-LAS at different Na^+ and Ca^{2+} concentrations.

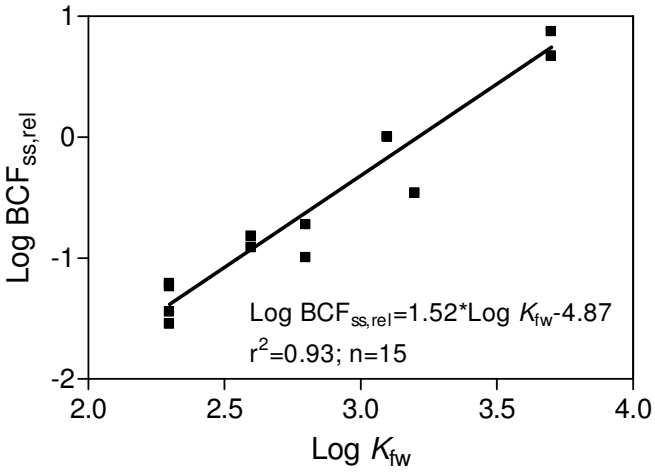

Figure S3. Relative Steady-state bioconcentration values (Reference compound: C_{12}-2-LAS) according to ref. (1) vs estimates of log K_{fw} from ref.(2).

Section 1. Discussion on sorption of LAS congeners to polyacrylate SPME fibers.

According to Jafvert *et al*. (*3*) the partitioning of an anionic organic compound to the octanol phase in a single electrolyte solution that contains divalent cations can be mainly described by the following reaction:

$M^{2+} + 2A^- = MA^+ + A^-$

Where M^{2+} represents the divalent cation and A^- is the organic anion. In this reaction, the anionic organic compound is acting as a counterion to maintain electroneutrality. When fitting the K_{fw} values and the log [Ca^{2+}] concentration from the simple electrolyte solution experiment to a sigmoidal curve with a fixed slope of 1, an apparent formation constant log ($K_{Ca(LAS)^+}$) of 2.5 is obtained. This value might be considered as an indication of the affinity of the partitioning of LAS at different Ca^{2+} concentration, but we cannot state if this is reflecting the real ion pair formation, since, to our knowledge, no formation constant of this complex is yet reported.

References

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(2) Rico-Rico, A.; Droge, S. T. J.; Widmer, D.; Hermens, J. L. M. Freely dissolved concentrations of anionic surfactants in seawater solutions: Optimization of the non-depletive solid-phase microextraction method and application to linear alkylbenzene sulfonates. *J. Chromatogr., A* **2009**, *1216*, 2996-3002.

(3) Jafvert, C. T.; Westall, J. C.; Grieder, E.; Schwarzenbach, R. P. Distribution of hydrophobic ionogenic organic compounds between octanol and water: Organic acids. *Environ. Sci. Technol.* **1990**, *24*, 1795-1803.