

Supporting Information for Comments on “Analysis of Narcotic Critical Body Residue Data using Equilibrium Distribution Concept and Refined Partition Coefficients”

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Contents

- Table S1 Polyparameter linear free energy relationship (PP-LFER) descriptors.
- Figure S1 Relative sorption capacities of individual biological components in *Hyalella azteca* (scud) and *Poecilia reticulata* (guppy).
- Figure S2 CBR_{wet} and CBR_{membrane} estimated with four sets of partition coefficients.

Table S1. Polyparameter linear free energy relationship (PP-LFER) descriptors.

	CAS-RN	E	S	A	B	V
1,2,4-Trichlorobenzene	120-82-1	0.98	0.81	0.00	0.00	1.084
1,2,3,4-Tetrachlorobenzene	634-66-2	1.18	0.92	0.00	0.00	1.206
n-Pentylbenzene	538-68-1	0.59	0.51	0.00	0.15	1.421
2,3,4-Trichloroaniline	634-67-3	1.24	1.20	0.35	0.15	1.183
2,3,5,6-Tetrachloroaniline	3481-20-7	1.31	1.34	0.46	0.03	1.306
4-Chloro-3-methylphenol	59-50-7	0.92	1.02	0.65	0.23	1.038

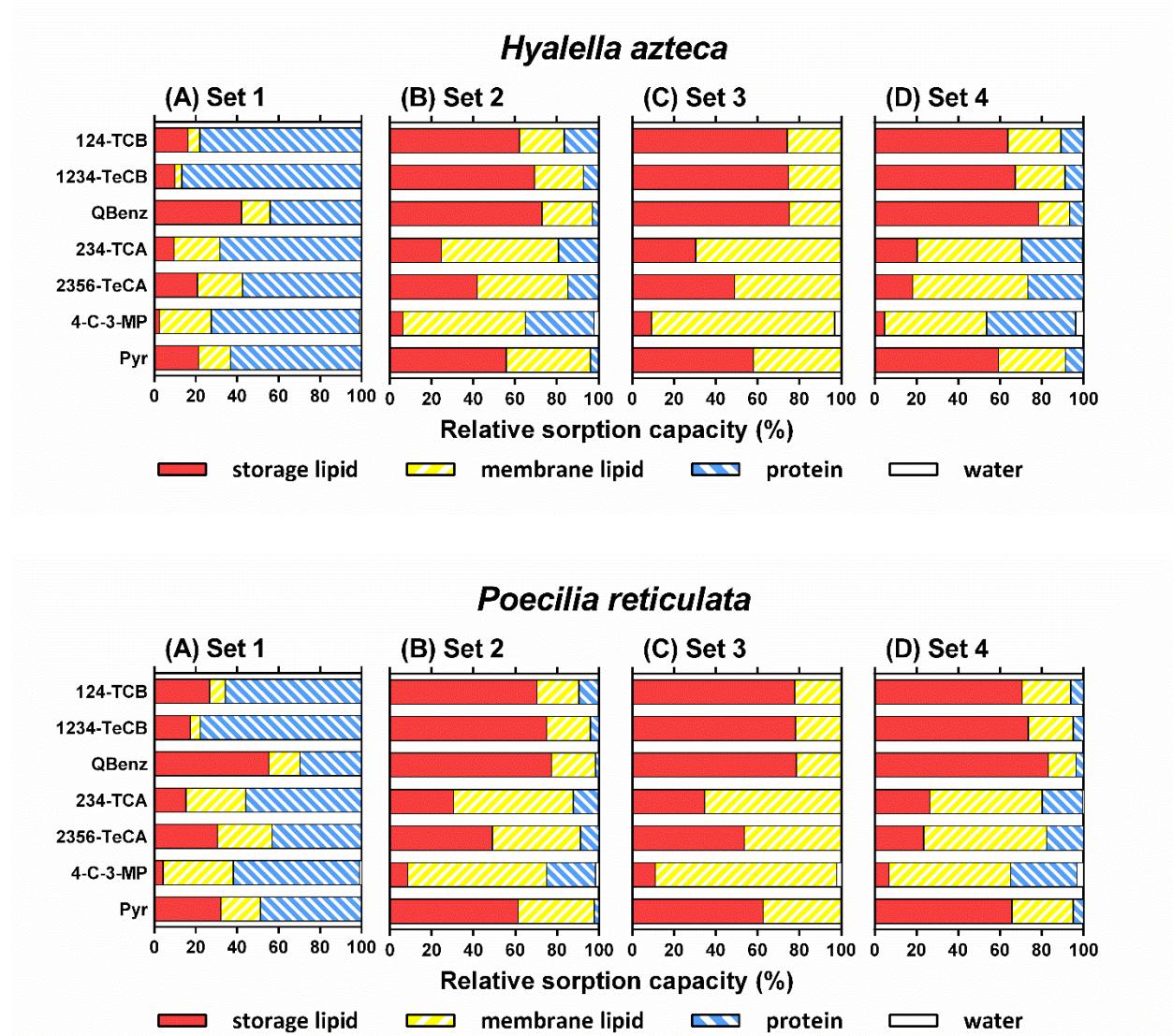


Figure S1. Relative sorption capacities of individual biological components in *Hyalella azteca* (scud) and *Poecilia reticulata* (guppy). The partition coefficients used for this calculation are summarized in Fig. 1. See Table 1 for the abbreviations of chemicals.

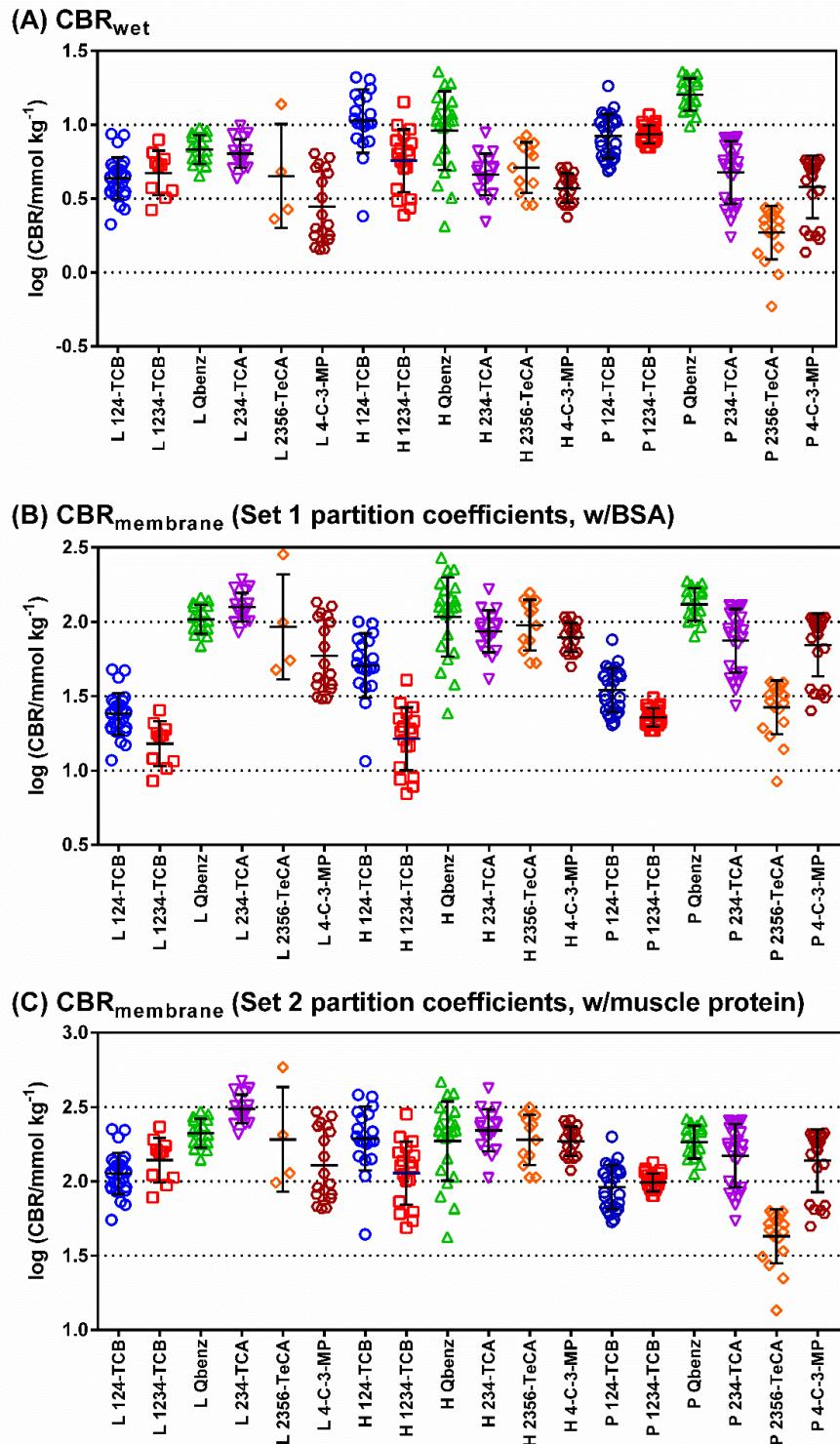
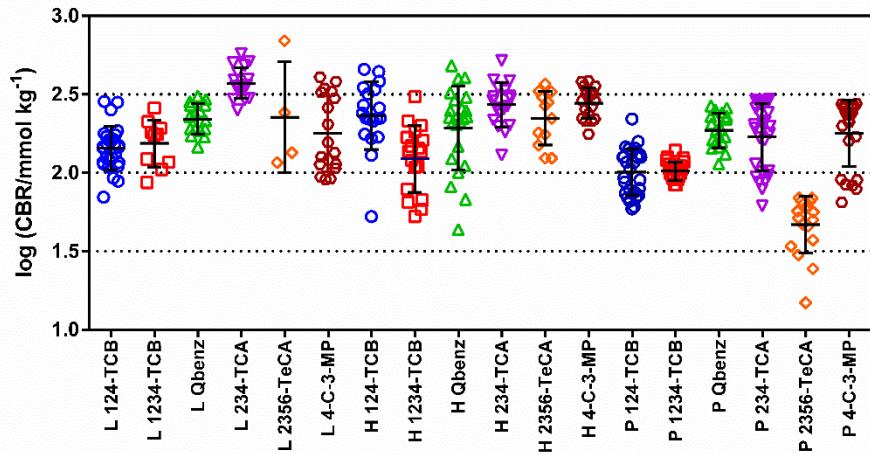


Figure S2. CBR_{wet} and $\text{CBR}_{\text{membrane}}$ estimated with four sets of partition coefficients. “L”, “H”, and “P” indicate *Lumbriculus variegatus*, *Hyalella Azteca*, and *Poecilia reticulata*, respectively. The original data are from van der Heijden et al.¹ The mean and the standard deviation are indicated with bars. Continued on next page.

(D) CBR_{membrane} (Set 3 partition coefficients, w/o protein)



(E) CBR_{membrane} (Set 4 partition coefficients, PP-LFERs)

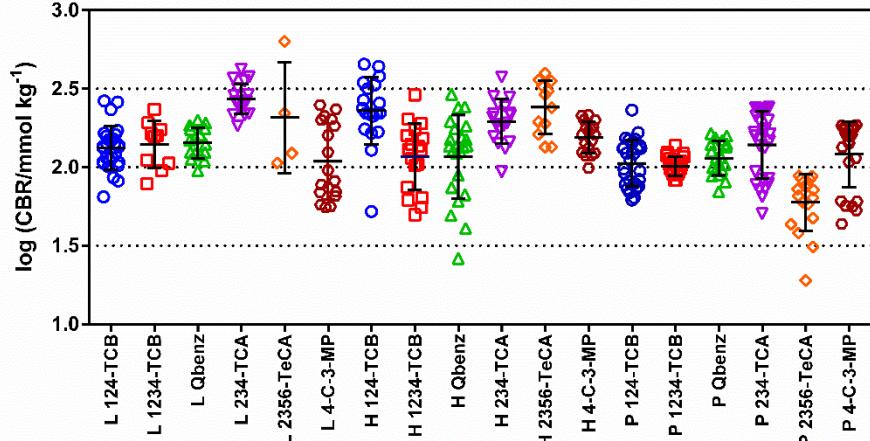


Figure S2. (Continued from previous page)

Reference in the Supporting Information

1. van der Heijden, S. A.; Hermens, J. L. M.; Sinnige, T. L.; Mayer, P.; Gilbert, D.; Jonker, M. T. O., Determining High-Quality Critical Body Residues for Multiple Species and Chemicals by Applying Improved Experimental Design and Data Interpretation Concepts. *Environ. Sci. Technol.* **2015**, *49*, (3), 1879-1887.