

Supporting Information

Title: Bioaccumulation of estrogenic hormones and UV-filters in red swamp crayfish (*Procambarus clarkii*)

Authors: Ke He ¹, Ethan Hain ¹, Anne Timm ², and Lee Blaney ^{*1}

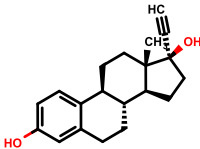
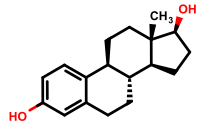
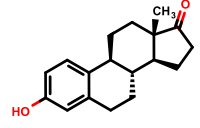
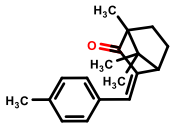
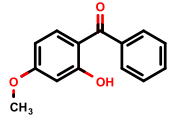
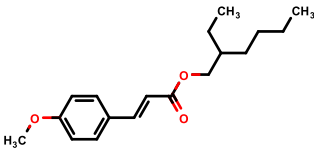
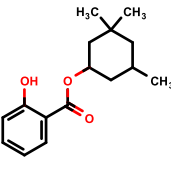
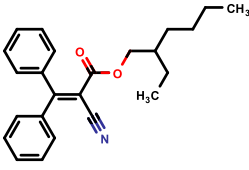
Affiliation: 1: University of Maryland Baltimore County
Department of Chemical, Biochemical, and Environmental Engineering
1000 Hilltop Circle, Engineering 314
Baltimore, MD 21250, USA

2: USDA Forest Service
Northern Research Station
5523 Research Park Drive, Suite 350
Baltimore, MD 21228, USA

* Corresponding Author: Lee Blaney, PhD
University of Maryland Baltimore County
Department of Chemical, Biochemical and Environmental Engineering
1000 Hilltop Circle, Engineering 314
Baltimore, MD 21250-0002, USA
Phone: (410) 455-8608
Fax: (410) 455-1049
Email: blaney@umbc.edu

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Table S1. Salient physicochemical properties of the three estrogens and five UV-filters.

Compound	Acronym	Chemical formula	Molecular weight (Da)	pK _a ^a	log D ^a	Structure
17 α -ethinylestradiol	EE2	C ₂₀ H ₂₄ O ₂	296.4	10.3	3.9	
17 β -estradiol	E2	C ₁₈ H ₂₄ O ₂	272.4	10.3	3.7	
Estrone	E1	C ₁₈ H ₂₂ O ₂	270.4	10.3	4.3	
4-methylbenzylidene camphor	4-MBC	C ₁₈ H ₂₂ O	254.4	n.a. ^b	5.1	
Benzophenone-3	BP-3	C ₁₄ H ₁₂ O ₃	228.2	7.1	2.7	
2-ethylhexyl-4-methoxycinnamate	EHMC	C ₁₈ H ₂₆ O ₃	290.4	n.a.	5.4	
Homosalate	HMS	C ₁₆ H ₂₂ O ₃	262.4	n.a.	5.0	
Octocrylene	OC	C ₂₄ H ₂₇ NO ₂	361.5	n.a.	6.7	

a: values estimated by MarvinSketch (ChemAxon, 2018); log D reported for pH 8.0

b: not applicable

Table S2. Results of the statistical analyses (as *p* values) for comparison of aqueous- and tail tissue-phase concentrations as a function of treatment (*i.e.*, Tanks 1, 2), time, and crayfish sex. Values lower than 0.05 indicate a significant difference between the factor levels identified for each parameter.

Parameter	Factor levels	<i>p</i> values for Student's t test							
		EE2	E2	E1	BP-3	4-MBC	OC	EHMC	HMS
Aqueous-phase concentrations during exposure period	10 min to 36 h (Tank 1)	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.157	0.935	0.506
	10 min to 36 h (Tank 2)	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.003	0.157	0.231
Parameter	Factor levels	<i>p</i> values for one-way ANOVA							
		EE2	E2	E1	BP-3	4-MBC	OC	EHMC	HMS
Aqueous-phase concentrations during elimination period (Tank 1)	Day 2 to Day 0	< 0.001	- ^a	- ^a	0.006	< 0.001	0.004	0.021	0.351
	Day 6 to Day 0	< 0.001	- ^a	- ^a	0.005	- ^a	0.014	0.719	0.954
	Day 10 to Day 0	< 0.001	- ^a	- ^a	0.004	- ^a	0.284	0.008	0.357
	Day 14 to Day 0	- ^a	- ^a	- ^a	0.002	- ^a	0.128	0.638	0.616
Aqueous-phase concentrations during elimination period (Tank 2)	Day 2 to Day 0	0.002	- ^a	- ^a	< 0.001	0.007	< 0.001	0.099	0.348
	Day 6 to Day 0	< 0.001	- ^a	- ^a	< 0.001	< 0.001	< 0.001	0.410	0.892
	Day 10 to Day 0	< 0.001	- ^a	- ^a	< 0.001	< 0.001	< 0.001	0.711	0.789
	Day 14 to Day 0	< 0.001	- ^a	- ^a	< 0.001	< 0.001	< 0.001	0.397	0.351
Parameter	Factor levels	<i>p</i> values for three-way ANOVA							
		EE2	E2	E1	BP-3	4-MBC	OC	EHMC	HMS
Tissue-phase concentrations for exposure and elimination periods	Female to male	- ^a	0.351	- ^a	0.920	0.210	0.309	0.053	0.822
	Day 28 to Day 14	- ^a	0.018	- ^a	0.906	< 0.001	0.005	0.939	0.176
	Day 42 to Day 14	- ^a	< 0.001	- ^a	0.810	< 0.001	< 0.001	0.052	0.054
	Day 56 to Day 14	- ^a	< 0.001	- ^a	< 0.001	- ^a	0.489	0.394	0.034
	Tank 2 to Tank 1	- ^a	< 0.001	- ^a	< 0.001	- ^b	< 0.001	< 0.001	< 0.001

a: The concentration was below its corresponding limit of detection and not included in the statistical analysis

b: 4-MBC was only detected in the tissue samples from Tank 2

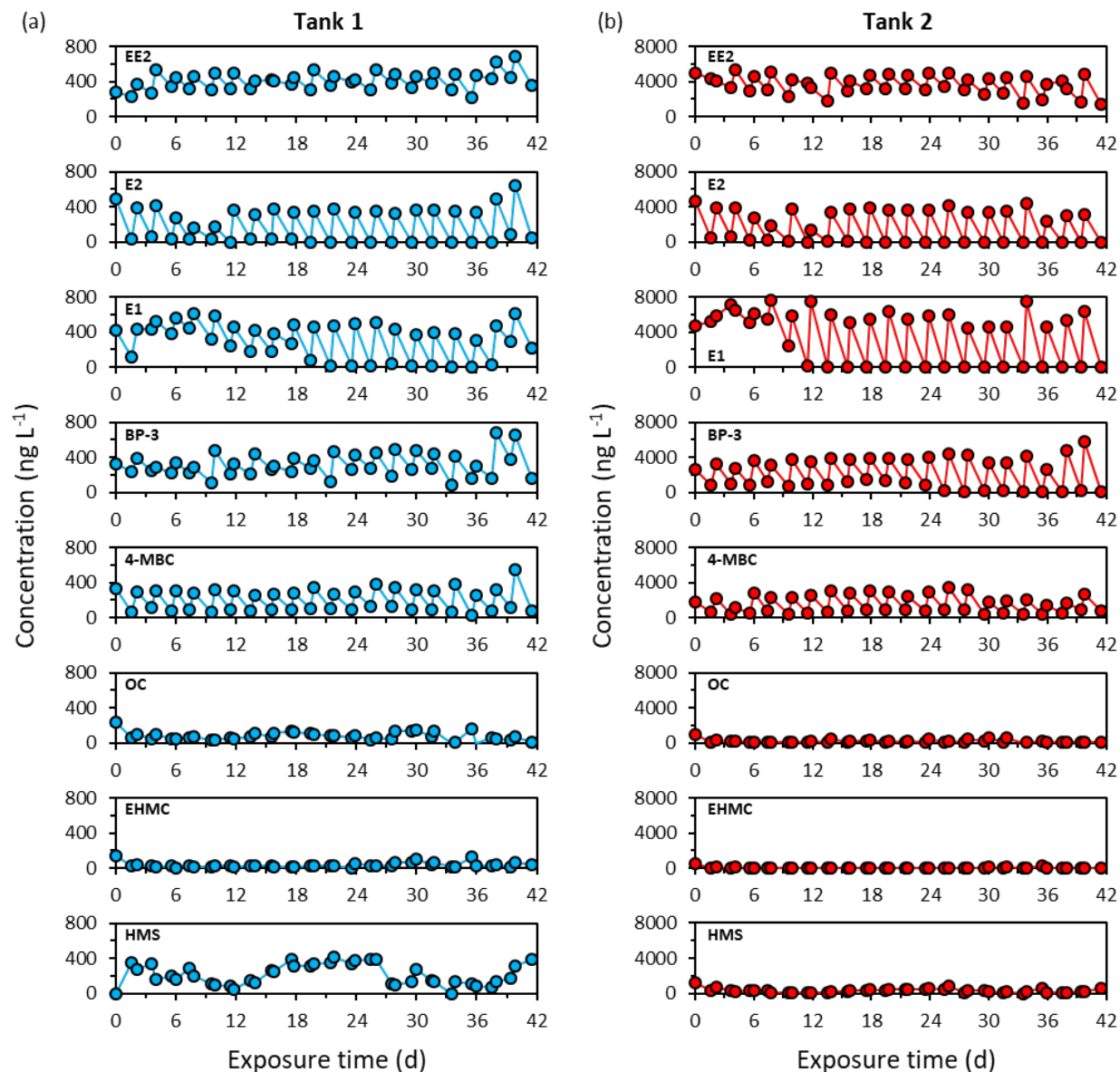


Figure S1. Measured EDC concentrations from water samples collected at the 10-min and 36-h sampling times in (a) Tank 1 and (b) Tank 2 during the 42-d exposure period. Analytes were dosed (according to mass balance analyses) every two days to reestablish the target conditions of 500 ng L⁻¹ in Tank 1 and 5000 ng L⁻¹ in Tank 2. Compounds are listed from top-to-bottom according to their retention time on the LC column, a parameter that is directly related to hydrophobicity. Note that the y-axis scales are held constant for each tank to highlight trends in aqueous-phase concentrations with hydrophobicity.

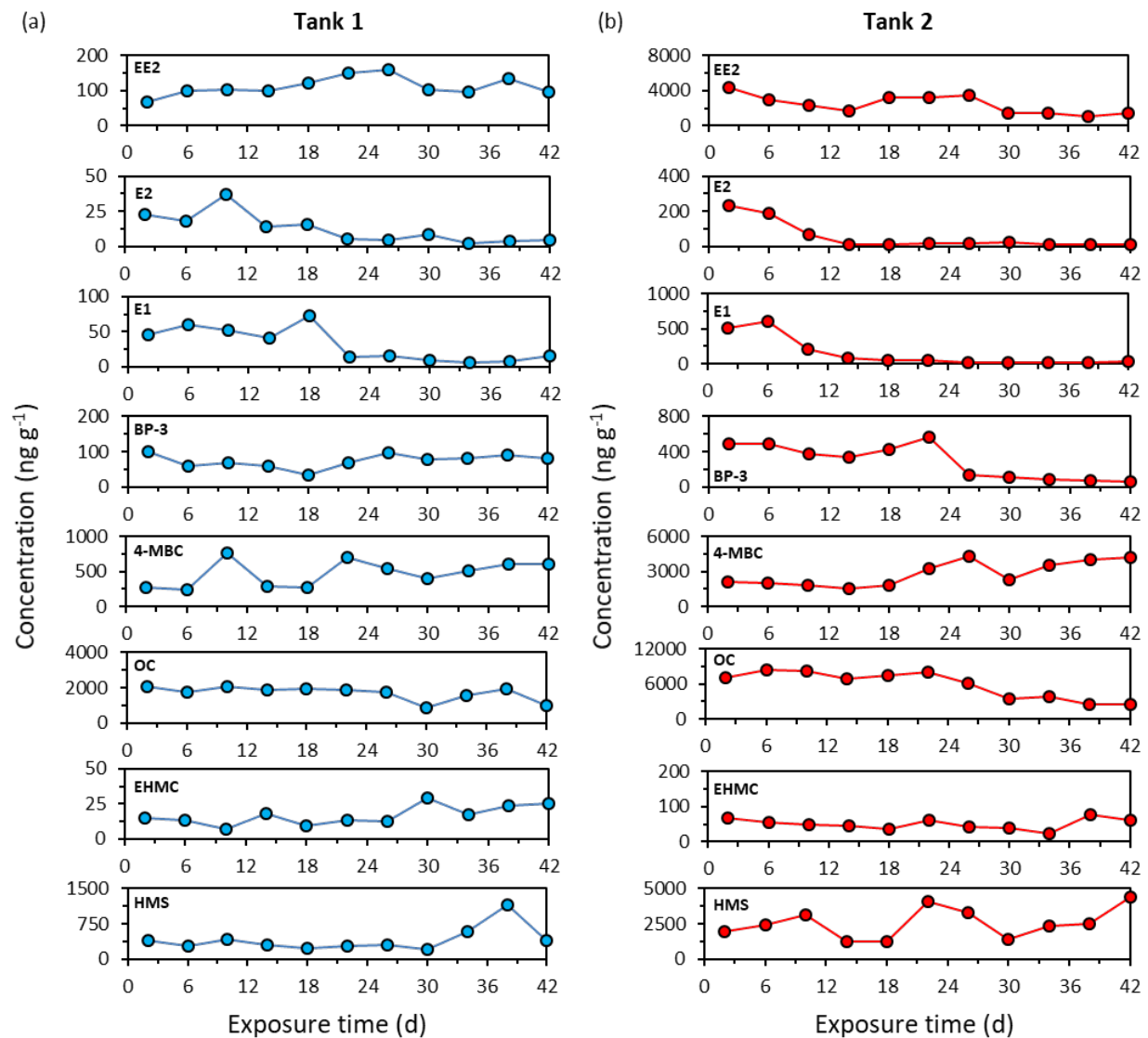


Figure S2. Measured EDC concentrations in the fecal matter collected from (a) Tank 1 and (b) Tank 2 during the 42-d exposure period. Fecal matter samples were collected every four days starting from the beginning of the acclimation period, but the data in the figure focus on Day 2 through Day 42 of the exposure period. Note that the y-axis scales are different for each tank and EDC due to the wide variation in fecal matter concentrations.

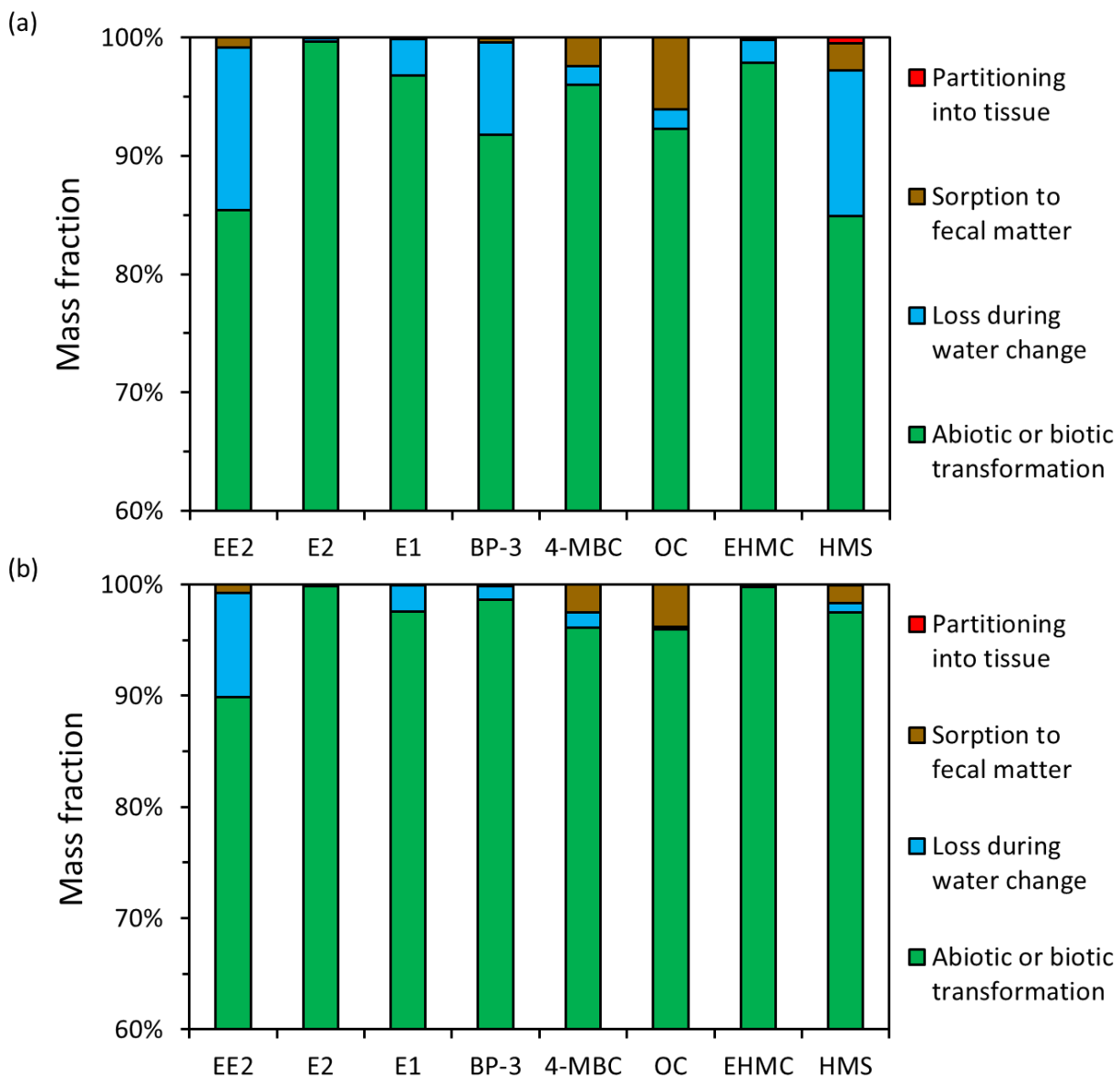


Figure S3. Mass balance analysis for (a) Tank 1 and (b) Tank 2 showing the contribution of various mechanisms (*i.e.*, partitioning into crayfish tail tissue, sorption to fecal matter, water change, and transformation) to EDC loss from the system during the 42-day exposure period.