Supporting Information

Sorption and Transport of Trenbolone and Altrenogest Photoproducts in Soil-Water Systems

Xingjian Yang[†,§,⊥,a], Haoqi Zhao[§,⊥,a], David M. Cwiertny[‖], Edward P. Kolodziej[*,‡,§,⊥]

[†]College of Natural Resources and Environment, South China Agricultural University, Guangzhou, PR China

[§]Department of Civil and Environmental Engineering, University of Washington, Seattle, Washington 98195, United States

[⊥]Center for Urban Waters, Tacoma, Washington 98421, United States

[‖]Department of Civil and Environmental Engineering, University of Iowa, Iowa City, Iowa 52242, United States

[‡]Interdisciplinary Arts and Sciences, University of Washington Tacoma, Tacoma, Washington 98421, United States

[a]The co-first authors contributed equally to this study

*Corresponding author at: Department of Civil and Environmental Engineering, University of Washington, Seattle, Washington 98195, United States; Interdisciplinary Arts and Sciences, University of Washington Tacoma, Tacoma, Washington 98402, United States; Center for Urban Waters, Tacoma, Washington 98421, United States. Tel: (253) 692-5659. E-mail address: koloj@uw.edu (E. P.

Kolodziej)

Materials. 17α-TBOH was obtained from BDG Synthesis (Wellington, New Zealand). 17β-TBOH was obtained from Shenzhen Shijingu Technology Co. Ltd (Shenzhen, China). TBO was purchased from Steraloids Inc (Newport, RI, USA). ALT and sodium bromide hydrate ($NaBr \cdot H_2O$, purity ≥ 99.9%) were purchased from Sigma Aldrich, Inc (St. Louis, MO, USA). Deuterated 17β-TBOH (17β-d_3-TBOH) used as internal standard was obtained from the Bank of Reference Standards (RIVM, Netherlands). Purities of all analytical standards were ≥ 95%. 1000 mg/L stock solutions of the steroids were prepared in methanol and stored at -20 °C. UHPLC grade methanol, toluene and water were purchased from Fisher Scientific (Pittsburgh, PA, USA). Dichloro-dimethylsiloxane (> 99%) was purchased from Acros Organics (Geel, Belgium). All glassware was silanized with a dichloro-dimethylsiloxane/toluene solution (1:9, *v:v*) prior to use.

Photoproduct production and quantification. The production and quantification methods for photoproducts are described in detail in our earlier work.[1] Briefly, photoproducts were generated using a solar simulator (EYE Lighting Int. Model # 93510, EYE Lighting, Mentor, OH) with four high pressure, 150 W xenon bulbs (Solarlux 150R, EYE Lighting, Mentor, OH). Aqueous solutions of the parent compounds (0.05-100 μg/L) were irradiated in clear borosilicate glass tubes for 6 hours (>99% conversion to photoproducts)[2-4] partially immersed in a chilled recirculating water bath (8-10 ˚C). For calibration standards of the photoproducts, 500

46 μL of the photoproduct solution was spiked with 0.5 ng of 17β-d_3-TBOH. Solutions
47 were then diluted (1:1 *v:v*) with methanol to enhance chromatography and
48 immediately analyzed via LC/MS/MS.
49 Photoproduct concentrations in the calibration standards were estimated based on
50 photoreaction yields reported in our previous studies,[3,4] specifically 73.3% and 6.7%
51 for 5-OH-17α-TBOH and 12-OH-17α-TBOH, 20% and 60% for 5-OH-17β-TBOH
52 and 12-OH-17β-TBOH, and 80% for TBO-OH and 80% for ALT-CAP-OH. To
53 produce and quantify ALT-CAP, ALT solutions were irradiated for ~3 minutes when
54 >95% of the parent mass was converted to ALT-CAP with partial conversion to ALT-
55 CAP-OH. The mass of residual ALT in samples was subtracted from the initial ALT
56 mass, and the remaining mass was allocated to ALT-CAP and ALT-CAP-OH based
57 on the ratio of their peak areas and prior observations on their near identical peak area
58 response via LC/MS/MS detection (data not shown). Photoproduct concentrations in
59 samples were then calculated via isotope dilution method. Calibration curves (~0.1-
60 100 μg/L) were built on a log-log scale in this study to ensure equal weight of each
61 data point in regression analysis (Figure S5).
62 Parents and related photoproducts were quantified by an Agilent 1290 HPLC
63 coupled to an Agilent 6460 mass spectrometer. The LC used an Agilent Poroshell
64 120Å EC C18 column (50 × 3.0 mm, 2.7μm) and a Gemini C18 guard column (4 mm
65 × 2.0 mm) (Phenomenex, USA) with LC-MS grade methanol and water (gradient
66 elution mode, 0.2 mL/min) as the mobile phase. To reduce heat-accelerated

67 photoproduct dehydration during analysis, the autosampler tray and chromatographic
68 columns were maintained at 4 ˚C and 10 ˚C, respectively. The multiple reaction
69 monitoring transitions and retention times of analytes are shown in Table S9 and other
70 instrumental details can be found in our previous study.[1]

71 ***K_{ow}* and *K_{hw}* measurement.** Octanol and hexane were extracted with 0.1 M
72 NaOH and rinsed twice with ultra-pure water. The solvents were then passed through
73 sodium sulfate (~0.5 g) (held on a layer of 0.2 μm glass fiber filter) to remove residual
74 water. 1 mL of octanol or hexane was then mixed with 3 mL of 10 mg/L aqueous
75 solutions (in Milli Q water) of the target steroids, and the mixture was equilibrated on
76 a shaker table (200 rmp, 24 hours). Upon equilibration, the samples were centrifuged
77 (3000 rpm, 1 h), after which subsamples of the organic phase and aqueous phase were
78 collected with glass pipettes. The samples were further diluted (organic phase with
79 methanol and aqueous phase with water) into linear ranges of the respective
80 calibration curves for LC-MS/MS analysis. For K_{ow} measurement of parent
81 compounds, octanol was diluted 500X and water was analyzed directly. For K_{hw}
82 measurement of parent compounds, hexane and water were diluted 500X and 1000X,
83 respectively. Octanol and water were diluted 500X and 20X in K_{ow} measurement of
84 photoproducts, and hexane and water were diluted 0.1X and 100X in K_{hw}
85 measurement of photoproducts, respectively.

86 **Batch Sorption Isotherms.** Linear isotherm (i.e., Equation (S1)) was used to fit
87 the batch sorption data

88 $$C_s = K_d \times C_w \quad \text{(S1)}$$

89 where C_s, C_w were steroid concentrations of sorbed and aqueous phases, respectively.

90 K_d (L/kg) is the linear distribution coefficient. K_d was then normalized to organic

91 carbon content (f_{oc}) of the soil-sand mixture to produce K_{oc} (Equation (S2))

92 $$K_{oc} = \frac{K_d}{f_{oc}} \quad \text{(S2)}.$$

93 **Transport modelling.** Column transport parameters were estimated with

94 CXTFIT 2.1 program,[5] which models solute transport by an equilibrium convection-

95 dispersion equation (CDE) that assumes one-dimensional transport of reactive solutes

96 subject to adsorption, first-order degradation, and zero-order production in a

97 homogeneous soil. The dimensionless form of the CDE equation can be written as:

98 The dimensionless form of the CDE equation can be written as:

99 $$R\frac{\partial C}{\partial T} = \frac{1\partial^2 C}{P\partial Z^2} - \frac{\partial C}{\partial Z} - \mu^E C + \gamma^E(Z) \quad \text{(S5)}$$

100 where $C = c/c_0$, $T = vt/L$, $Z = x/L$, $P = vL/D$, $\mu^E = \mu L/v$, and $\gamma^E = \gamma L/vc_0$ are

101 dimensionless. c is the concentration in the liquid phase (μg/L), x and t are distance

102 (cm) and time (min), respectively. D represents the dispersion coefficient (cm^2/min), v

103 is the pore water velocity (cm/min), μ is the first-order decay coefficient for solute

104 degradation (min^{-1}), and γ is the zero-order production coefficient (cm^{-1}). c_0 and L are

105 the characteristic concentration (μg/L) and length (cm), respectively. R represents the

106 retardation factor.

107 CXTFIT can also model non-equilibrium transport. Physical non-equilibrium is

modelled by partitioning the liquid phase into mobile and stagnant regions. In contrast, chemical non-equilibrium is considered as a two-site system, which assumes that some of the sites (type-1 sites) are at equilibrium while type-2 sites represent kinetically limited adsorption sites. The chemical and physical non-equilibrium models can be reduced to a same form when using dimensionless parameters:

$$\beta R\frac{\partial C_1}{\partial T} = \frac{1}{P}\frac{\partial^2 C_1}{\partial Z^2} - \frac{\partial C_1}{\partial Z} - \omega(C_1 - C_2) \quad \text{(S6)}$$

where subscripts 1 and 2 refer to equilibrium and non-equilibrium sites, respectively. β is a partitioning coefficient and ω is a dimensionless mass transfer coefficient. For two-sites non-equilibrium model, β represents the fraction of "Type-1" sites contributing to instantaneous sorption, ω represents ratio of column hydraulic retention time to timescales for chemical partitioning. C_1 and C_2 represent the dimensionless solute concentration in equilibrium and nonequilibrium sites, respectively. P is the Peclet number.

Quality assurance and quality control. To improve sensitivity and reduce formation of $[M+Na]^+$ adducts during ionization, all glassware was rinsed with ultrapure water and methanol for three times and silanized prior to use. Solute retention times (within 2%) and the relative abundance (within 20%) of two selected MRM transitions needed to match analytical standards. Isotope dilution quantification was used to account for sample preparation, matrix effect, and instrumental response variation. Method detection limit (MDL) was defined as standard concentration where signal-to-noise ratio of 3 was observed, respectively. MDLs for parent steroids were

129 0.006-0.14 μg/L, and for photoproducts were 0.008-0.60 μg/L (Table S2). For column
130 studies, procedural blanks were conducted by quantifying solutes in column effluents
131 (N = 4) where model water (without steroids) was the input solution. No steroids or
132 interferences were detected in these trials. Then, matrix effect tests (N =8) were
133 conducted by spiking 10 μg/L of 17α-TBOH, ALT, and corresponding photoproducts
134 into column effluents. The matrix effect factors were evaluated as the peak area ratio
135 of analytes in column effluents to analytes in standard solutions, and were 66-85% for
136 17α-TBOH, ALT, and the photoproducts. The matrix effect factor for 17β-d3-TBOH
137 was 74%, which well matched the matrix effect factors of target analytes (Table S2).
138 Precision (N = 8) was evaluated as the relative standard deviations of triplicate
139 quantifications of one column effluent, and was 3-9% for 17α-TBOH, ALT, and the
140 photoproducts (Table S2).

References

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Table S1. Physical-chemical properties of model soil used in batch and column studies.

parameter		value	parameters		value
pH		6.36	metal content (μg/g)	K	827
organic carbon (%)		1.13		Mg	7120
CEC (meq/100 g)		11.5		Mn	393
total nitrogen (%)		0.086		Mo	31.1
metal content (μg/g)	Al	11400		Na	113
	As	ND[a]		Ni	46.1
	B	35.3		P	962
	Ba	49.2		Pb	48.4
	Ca	2870		S	215
	Cd	ND		Se	43.6
	Cr	23.3		Zn	60.4
	Cu	17.4		Si	353
	Fe	21400		Ag	ND

[a] ND = Not detected.

Table S2. Calibration curve linearity, method detection limits, matrix effect and precision in soil column experiments for the target compounds.

analyte	R^2	MDLs (μg/L)	matrix effect (%)	precision (%)
17α-TBOH	0.999	0.006	85	3
5-OH-17α-TBOH	0.999	0.37	75	7
12-OH-17α-TBOH	0.998	0.44	66	9
17β-TBOH	0.999	0.013	-	-
5-OH-17β-TBOH	0.998	0.52	-	-
12-OH-17β-TBOH	0.995	0.60	-	-
TBO	0.999	0.14	-	-
TBO-OH	0.999	0.17	-	-
ALT	0.999	0.022	83	8
ALT-CAP	0.999	0.008	68	6
ALT-CAP-OH	0.999	0.11	64	3
17β-d3-TBOH	-	-	74	-

Table S3. Isotherm data for TBA metabolites and ALT. Batch sorption was tested in duplicate experiments, plus a water control with no load of soil to test on the aqueous phase stability of TBA metabolites and ALT during equilibration period. C_{in} (μg/L), C_w (μg/L) and C_s (μg/kg) are input concentrations and concentrations in the aqueous and sorbed phases, respectively.

C_{in}		17α-TBOH			17β-TBOH			TBO			ALT		
		C_w	C_s	mass recovery (%)	C_w	C_s	mass recovery (%)	C_w	C_s	mass recovery (%)	C_w	C_s	mass recovery (%)
0.1	1	0.059	0.10	84	0.056	0.14	91	0.033	0.28	103	0.055	0.22	109
	2	0.096	0.10	121	0.033	0.13	65	0.048	0.22	104	0.050	0.21	103
	no-soil control	0.059	n.a.[a]	59	0.078	n.a.	78	0.031	n.a.	31	0.060	n.a.	60
0.5	1	0.34	0.54	94	-[b]	-	-	0.22	1.1	99	-	-	-
	2	0.33	0.72	102	-	-	-	0.25	1.2	112	-	-	-
	no-soil control	0.25	n.a.	51	-	-	-	0.22	n.a.	43	-	-	-
1	1	0.63	0.94	86	0.54	1.3	87	0.44	1.7	87	0.53	2.1	105
	2	0.66	1.1	93	0.52	1.2	83	0.43	2.7	109	0.51	1.8	95
	no-soil control	0.81	n.a.	81	0.85	n.a.	85	0.54	n.a.	54	1.0	n.a.	104
5	1	3.4	5.8	98	-	-	-	2.9	9.6	107	3.3	11	120
	2	3.5	5.6	98	-	-	-	3.1	9.9	111	2.9	7.7	96
	no-soil control	2.2	n.a.	45	-	-	-	3.3	n.a.	65	3.6	n.a.	73
10	1	6.3	14	99	7.2	11	100	5.3	16	93	5.1	17	94
	2	7.4	9.9	99	5.8	14	93	5.5	23	112	5.3	16	94
	no-soil control	7.5	n.a.	75	10	n.a.	102	3.5	n.a.	35	8.0	n.a.	80

[a] n.a.: not applicable. The control only contained aqueous phase.

[b] The sorption of 17β-TBOH was not tested under 0.5 μg/L and 5 μg/L, and the sorption of ALT was not tested under 0.5 μg/L, due to inconsistent experiment design for different batches of experiment.

Table S4. Isotherm data for photoproducts of TBA metabolites and ALT in static soil-water systems. Batch sorption was tested in duplicate which included a no-soil control and a dark control. C_{in}(μg/L), C_w (μg/L) and C_s (μg/kg) are input concentrations and concentrations in the aqueous and sorbed phases, respectively.

C_{in}		17α-TBOH photoproducts							17β-TBOH photoproducts						
		5-OH-17α-TBOH		12-OH-17α-TBOH		17α-TBOH		mass	5-OH-17β-TBOH		12-OH-17β-TBOH		17β-TBOH		mass
		C_w	C_s	C_w	C_s	C_w	C_s	recovery (%)	C_w	C_s	C_w	C_s	C_w	C_s	recovery (%)
1	1	0.80	0.39	ND[a]	ND	0.065	0.11	119	ND	ND	ND	ND	ND	ND	0
	2	0.82	0.46	ND	ND	0.074	0.12	117	ND	ND	ND	ND	ND	ND	0
	no-soil control	0.61	n.a.[b]	ND	n.a.	0.11	n.a.	76	ND	n.a.	ND	n.a.	ND	n.a.	0
	dark control	ND	ND	ND	ND	0.83	0.89	105	ND	ND	ND	ND	0.59	1.5	96
5	1	3.9	2.4	ND	ND	0.39	0.44	113	0.49	1.6	3.0	4.0	0.042	ND	122
	2	4.3	1.9	ND	ND	0.37	0.42	119	0.57	ND	2.4	ND	0	ND	74
	no-soil control	3.0	n.a.	ND	n.a.	0.47	n.a.	75	0.89	n.a.	2.1	n.a.	0.12	n.a.	74
	dark control	ND	ND	ND	ND	4.3	3.8	104	ND	ND	ND	ND	2.3	9.5	93
10	1	8.5	4.1	0.25	0.41	0.72	0.85	123	1.8	ND	6.0	ND	0.047	ND	99
	2	7.7	4.1	0.64	0.23	0.72	0.83	118	2.1	ND	5.6	ND	0.055	0.077	96
	no-soil control	5.9	n.a.	0.17	n.a.	1.5	n.a.	76	0.99	n.a.	3.3	n.a.	0.37	n.a.	54
	dark control	ND	ND	ND	ND	8.5	8.1	105	ND	ND	ND	ND	6.5	15	102
50	1	45	20	3.5	2.4	4.9	5.7	135	6.0	6.1	21	13	0.35	0.56	78
	2	44	23	3.3	4.0	3.6	5.4	135	7.6	6.3	13	21	0.39	0.81	70
	no-soil control	38	n.a.	2.8	n.a.	7.6	n.a.	101	4.8	n.a.	16	n.a.	1.5	n.a.	52
	dark control	ND	ND	ND	ND	43	39	105	ND	ND	ND	ND	32	69	98
100	1	85	39	6.1	4.4	8.8	10	127	13	13	50	36	0.61	1.8	94
	2	92	49	7.5	6.3	9.3	12	142	11	5.4	44	14	0.77	1.8	75
	no-soil control	86	n.a.	5.4	n.a.	21	n.a.	114	3.5	n.a.	11	n.a.	4.5	n.a.	18
	dark control	ND	ND	ND	ND	81	79	101	ND	ND	ND	ND	72	130	106

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C_{in}		TBO photoproducts					ALT-CAP							ALT-CAP-OH						
		TBO-OH		TBO		mass	ALT-CAP		ALT-CAP-OH		ALT		mass	ALT-CAP		ALT-CAP-OH		ALT		mass
		C_w	C_s	C_w	C_s	recovery (%)	C_w	C_s	C_w	C_s	C_w	C_s	recovery (%)	C_w	C_s	C_w	C_s	C_w	C_s	recovery (%)
1	1	2.0	ND	ND	ND	252	0.34	0.89	0.39	ND	0.019	0.076	99	0.089	ND	ND	ND	ND	ND	0
	2	ND[a]	ND	ND	ND	0	0.30	1.1	0.32	ND	0.015	0.056	93	0.097	ND	ND	ND	ND	ND	0
	no-soil control	1.1	n.a.[b]	ND	n.a.	143	0.47	n.a.	0.47	n.a.	0.039	n.a.	98	0.14	n.a.	0.33	n.a.	ND	n.a.	42
	dark control	ND	ND	0.32	2.9	104	ND	ND	ND	ND	0.25	1.0	51	ND	ND	ND	ND	0.25	1.0	51
5	1	6.2	11	0.071	0.54	220	2.1	4.2	2.2	1.2	0.11	0.29	117	0.46	0.56	1.2	1.8	ND	ND	40
	2	5.8	4.9	0.058	0.42	177	1.9	4.0	1.9	1.1	0.090	0.27	105	0.49	0.43	1.1	2.4	ND	ND	43
	no-soil control	4.5	n.a.	0.16	n.a.	113	2.5	n.a.	2.2	n.a.	0.20	n.a.	100	0.27	n.a.	4.1	n.a.	ND	n.a.	101
	dark control	ND	ND	3.0	12	119	ND	ND	ND	ND	1.5	7.2	66	ND	ND	ND	ND	1.5	7.2	66
10	1	10	8.6	0.14	1.2	153	4.4	6.7	4.1	2.2	0.23	0.55	110	0.99	1.9	7.3	7.0	ND	ND	113
	2	11	10	0.20	0.80	168	4.3	8.8	3.5	2.3	0.19	0.62	110	0.90	1.8	6.2	4.3	ND	ND	91
	no-soil control	8.8	n.a.	0.36	n.a.	109	5.4	n.a.	4.5	n.a.	0.46	n.a.	104	0.42	n.a.	8.1	n.a.	ND	n.a.	101
	dark control	ND	ND	8.0	20	131	ND	ND	ND	ND	3.5	9.6	59	ND	ND	ND	ND	3.5	9.6	59
50	1	45	49	0.98	5.8	143	22	50	19	13	1.1	4.0	117	4.0	7.7	37	25	ND	ND	108
	2	47	31	1.4	3.4	137	23	38	20	13	1.3	3.0	116	4.4	8.9	37	28	ND	ND	110
	no-soil control	42	n.a.	2.0	n.a.	105	21	n.a.	23	n.a.	1.9	n.a.	91	DATA MISSING						
	dark control	ND	ND	28	110	111	ND	ND	ND	ND	14	55	55	ND	ND	ND	ND	14	55	55
100	1	78	95	2.5	11	127	37	100	33	29	1.8	8.5	106	5.4	8.7	81	54	ND	ND	118
	2	75	68	2.2	12	115	40	80	37	24	2.3	6.6	107	13	38	69	52	ND	ND	103
	no-soil control	73	n.a.	4.1	n.a.	92	35	n.a.	44	n.a.	3.5	n.a.	82	4.8	n.a.	81	n.a.	ND	n.a.	101
	dark control	ND	ND	61	160	100	ND	ND	ND	ND	38	150	76	ND	ND	ND	ND	38	150	76

177 [a] ND: not detected;

178 [b] n.a.: not applicable. The no-soil control only contained aqueous phase.

Table S5. Observed mass distribution across water, soil, glass tubes, and tube caps when 0.1, 1, 10 μg/L of 17α-TBOH was spiked into glass tubes with water only or with soil and water.

	spiked levels (μg/L)	17α-TBOH mass (%)			
		water	soil	tube	cap
water only	0.1	49	-	56	0
	1	19	-	78	0
	10	28	-	59	0
soil-water system	0.1	66	16	0	0
	1	58	18	8	0
	10	52	14	30	0

Table S6. Physical properties of soil columns and estimated hydraulic parameters based upon bromide tracer data.

experiment #	column	recovery (%)	R^2	volumetric water content (θ) (cm^3/cm^3)	pore water velocity (v) (cm/min)[a]		bulk density (ρ_b) (g/mL)	dispersion coefficient (D) (cm^2/min)
					measured	estimated		
1	light	99	0.996	0.43	0.13	0.15	1.52	0.11
	dark control	100	0.997	0.40	0.12	0.15	1.58	0.07
2	light	100	0.997	0.37	0.16	0.18	1.67	0.13
	dark control	100	0.996	0.42	0.11	0.21	1.54	0.12
3	light	100	0.997	0.42	0.13	0.21	1.54	0.12
	dark control	100	0.997	0.38	0.15	0.21	1.65	0.12
4[b]	light	-	-	0.40	0.14	-	1.59	-
	dark control	-	-	0.42	0.12	-	1.53	-
5	light	100	0.997	0.42	0.14	0.18	1.53	0.13
	dark control	100	0.997	0.43	0.12	0.21	1.52	0.12
6	light	98	0.996	0.42	0.13	0.16	1.54	0.20
	dark control	99	0.996	0.41	0.13	0.15	1.56	0.15

[a] Measured velocity can be calculated as $v = Q/(A \times \theta)$, where Q and A is volumetric flow rate (cm^3/min) and cross-sectional area of the soil column (cm^2), respectively. Estimated v was obtained by CXTFIT program.

[b] Experiment #4 was conducted to assess solute reproducibility, no tracer test was done.

Table S7. Detailed transport parameters for parent compounds in CXTFIT model.[a]

experiment	column	compound	R_{mod}[b]	β	ω	R^2
1	dark	17β-TBOH	21.0	0.12	2.76	0.99
2	dark	17α-TBOH	14.1	0.19	1.34	0.99
		ALT	22.6	0.23	2.28	0.99
3	dark	17α-TBOH	14.8	0.16	1.57	0.99
		ALT	20.4	0.20	2.48	0.99
5	dark	17α-TBOH	13.7	0.18	1.29	0.96
		ALT	22.6	0.17	2.69	0.93
6	dark	ALT	25.4	NE[c]	NE	0.99

[a] The transport parameters were obtained by two-site non-equilibrium model.

[b] R_{mod} represents retardation factor obtained from modelling.

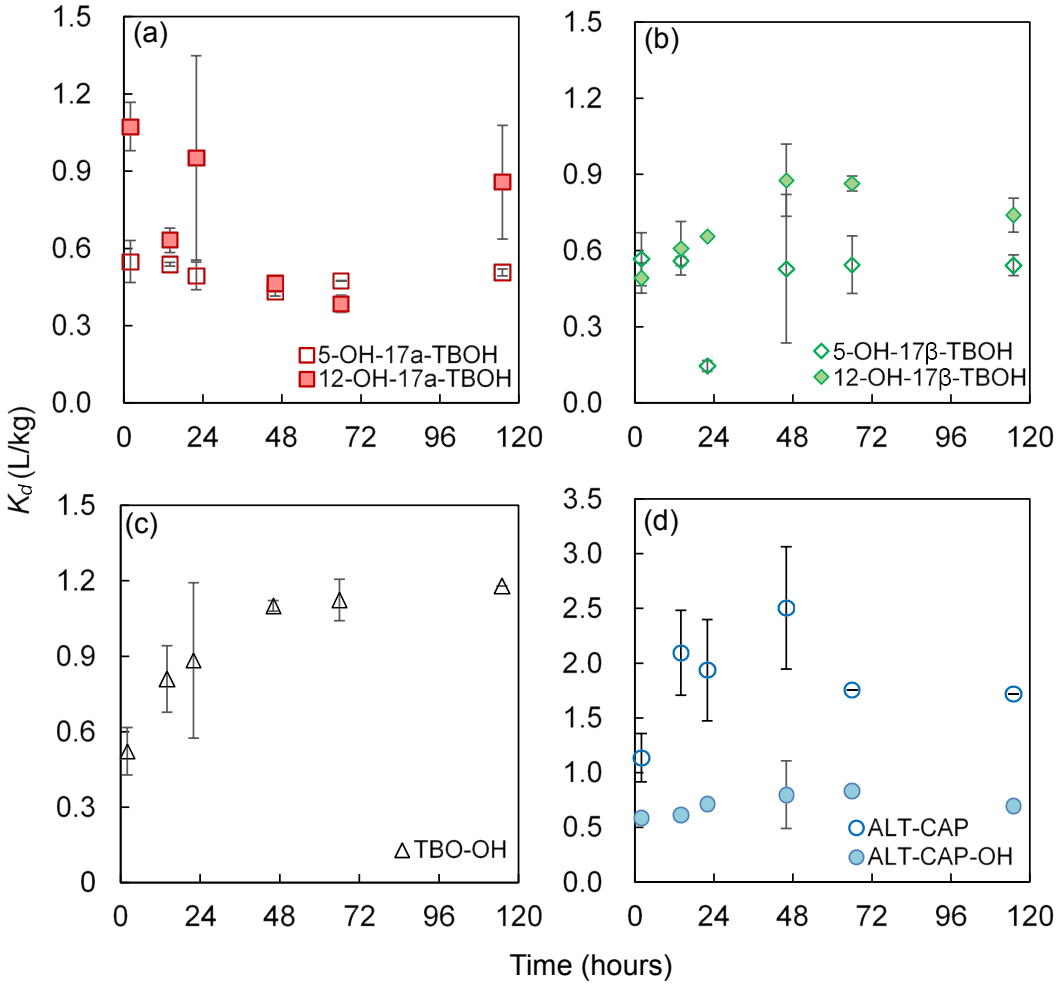
[c] NE = Not estimated.

Table S8. Fitted parameters for Br^- and solutes during modelling.

experiment	solute	model	fitted parameter
1-6	Br^-	Convection-dispersion model	v and D
1-6	17α-TBOH, ALT, 17β-TBOH, and their photoproducts	Two-Site	R_{mod}, β, and ω

Table S9. Elution times, multiple reaction monitoring (MRM) transitions, fragmenter voltages, and collision energies for TBA metabolites, altrenogest, and photoproducts in LC-MS/MS analysis.

compound	retention time (min)	MRM transitions (m/z)	fragmentor (V)	collision energy (eV)
17α-TBOH	7.55	271>253 (271>211)	135 (135)	30 (30)
5-OH-17α-TBOH	6.62	271>211 (271>253)	135 (135)	30 (30)
12-OH-17α-TBOH	7.13	271>211 (271>253)	135 (135)	30 (30)
17β-TBOH	7.23	271>253 (271>211)	135 (135)	30 (30)
5-OH-17β-TBOH	4.87	271>211 (271>253)	135 (135)	30 (30)
12-OH-17β-TBOH	5.85	271>211 (271>253)	135 (135)	30 (30)
TBO	6.65	269>225 (269>169)	135 (135)	28 (28)
TBO-OH	5.14	269>169 (269>225)	135 (135)	28 (28)
ALT	9.37	311>227 (311>269)	82 (82)	24 (12)
ALT-CAP	8.41	311>269 (311>227)	82 (82)	12 (24)
ALT-CAP-OH	5.43	311>269 (311>227)	82 (82)	12 (24)
17β-d_3-TBOH	7.26	274>256 (274>214)	135 (135)	30 (30)



197

198 **Figure S1.** The partitioning coefficients in single concentration (~50 μg/L as parents
199 before irradiation) time series study for (a) 17α-TBOH, (b) 17β-TBOH, (c) TBO and
200 (d) ALT photoproducts. Sorption was tested in duplicates at each time spot. The
201 sorption system generally reaches equilibrium at 22 hours. Error bars represent
202 standard deviations.

203

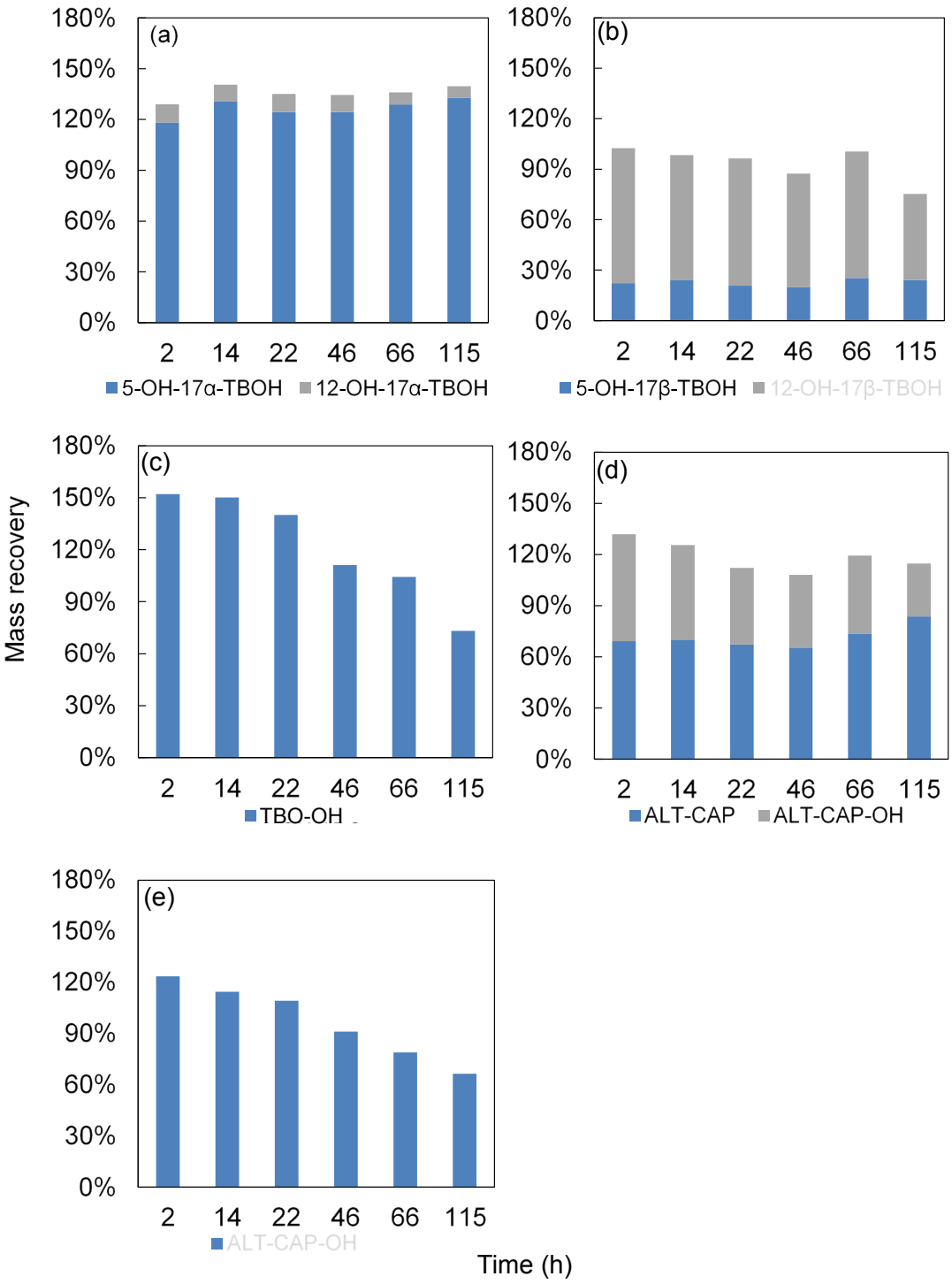


Figure S2. The mass recoveries in single concentration (~50 μg/L as parents before irradiation) time series study for (a) 17α-TBOH, (b) 17β-TBOH, (c) TBO (d) ALT and (e) ALT-CAP photoproducts. Product-to-parent reversion was observed for ALT-CAP-OH. Mass recoveries were calculated as the mass ratio of photoproducts detected over the photoproducts spiked.

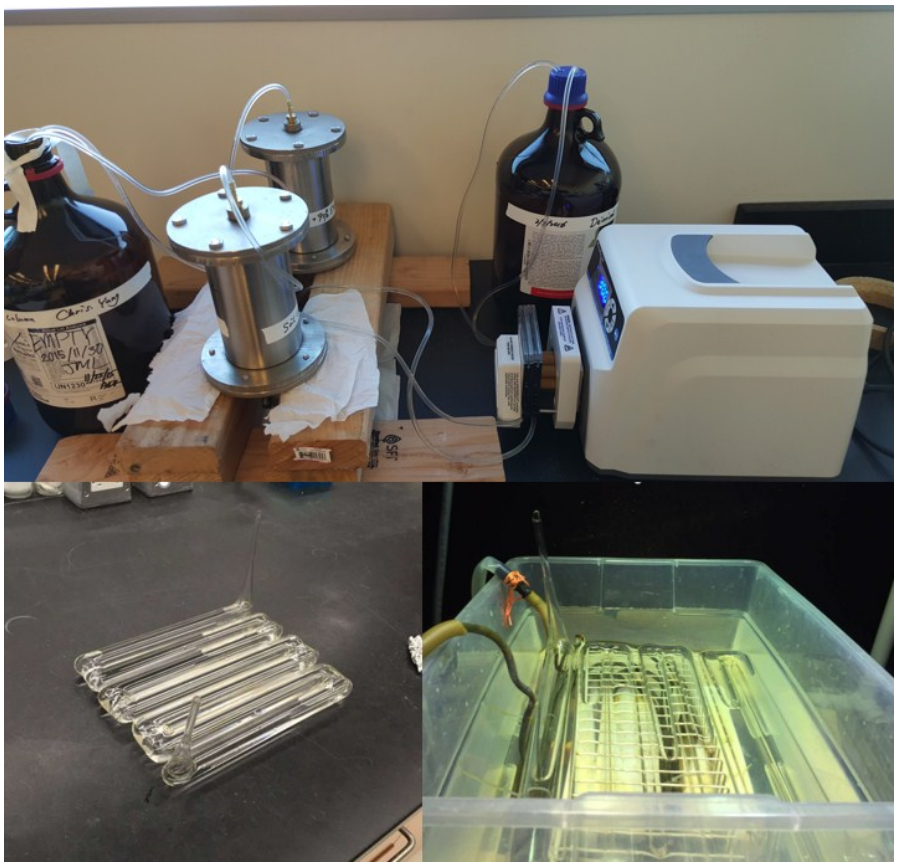


Figure S3. Photographs of soil column and glass coil.

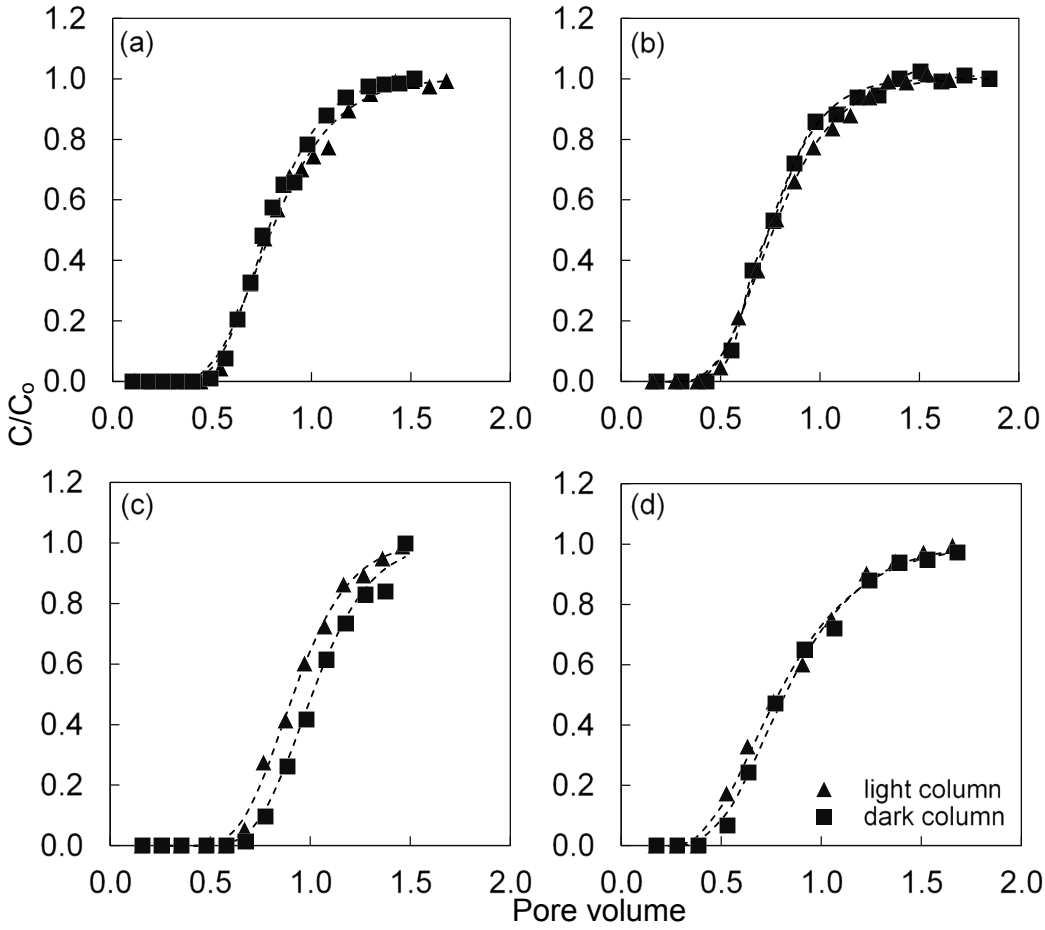


Figure S4. Bromide tracer tests for (a) short-term transport of 17β-TBOH in dark control column, and 17β-TBOH, 5-OH-17β-TBOH, and 12-OH-17β-TBOH transport in light columns; (b) short-term transport of 17α-TBOH in dark control column, and 17α-TBOH, 5-OH-17α-TBOH, and 12-OH-17α-TBOH in light columns; (c) long-term transport of 17α-TBOH in dark control column, and 17α-TBOH, 5-OH-17α-TBOH, and 12-OH-17α-TBOH in light columns; and (d) long-term transport of ALT in dark control columns, and ALT, ALT-CAP, and ALT-CAP-OH in light columns.

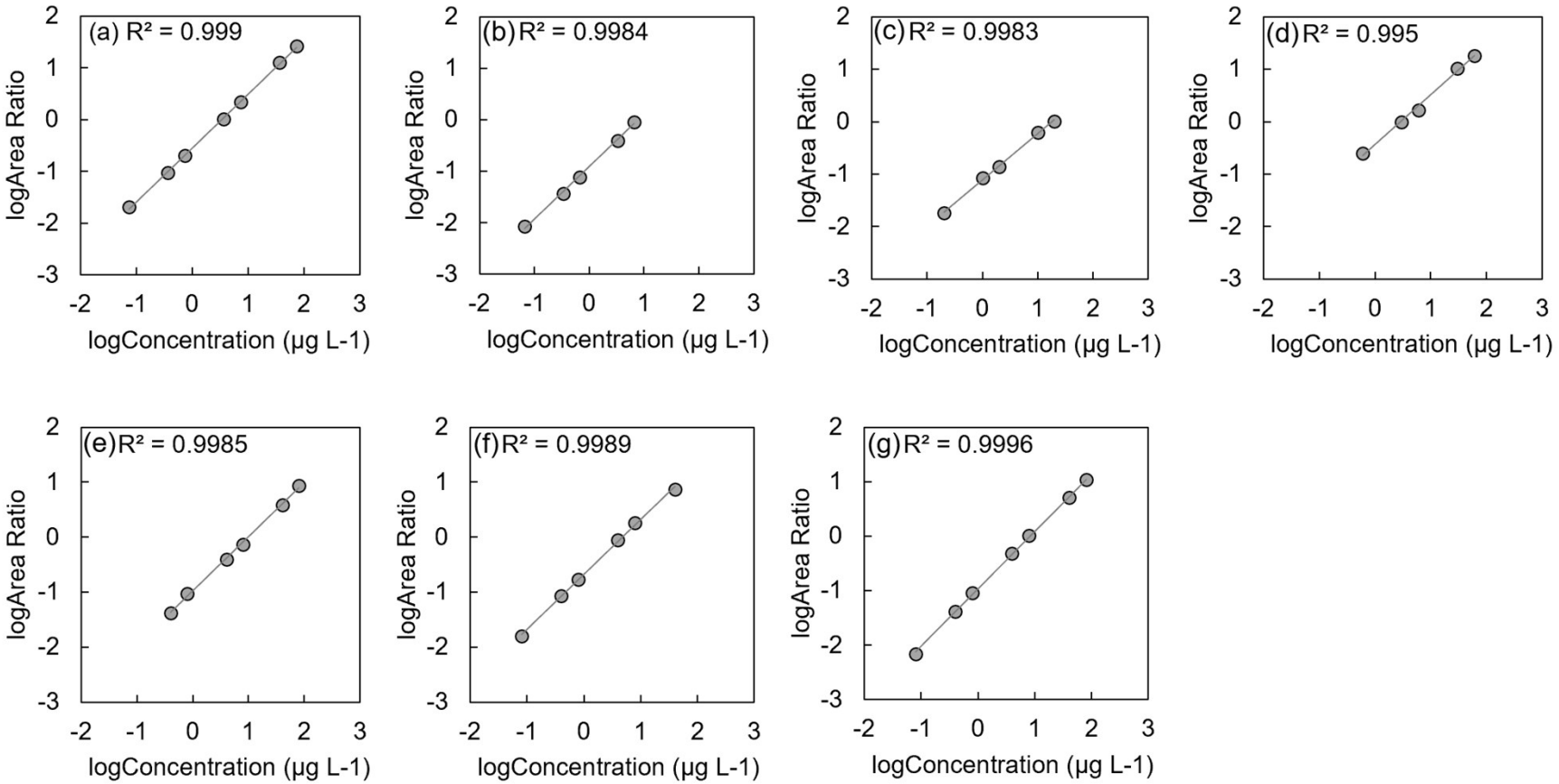


Figure S5. Calibration curves of (a) 5-OH-17α-TBOH, (b) 12-OH-17α-TBOH, (c) 5-OH-17β-TBOH, (d) 12-OH-17β-TBOH, (e) TBO-OH, (f) ALT-CAP, (g) ALT-CAP-OH at 0.1-100 µg L^{-1} as parent concentrations before irradiation, corresponding to 0.073-73 ug L^{-1} for 5-OH-17α-TBOH, 0.0067-6.7 µg L^{-1} for 12-OH-17α-TBOH, 0.02-20 µg L^{-1} for 5-OH-17β-TBOH, 0.06-60 µg L^{-1} for 12-OH-17β-TBOH, and 0.08-80 µg L^{-1} for TBO-OH, ALT-CAP, and ALT-CAP-OH. When observed, calibration curves with fewer than seven data points represent no detection of the analytes at low concentrations. Area ratio refers to ratio of the LC-MS/MS peak areas of the analytes over that of the isotopic internal standard. The data was first presented in Kenyon et al. (2019)