

SUPPORTING INFORMATION

Partitioning of Fluorotelomer Alcohols to Octanol and Different Sources of Dissolved Organic Carbon

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Estimation of Percent Aromatic Carbon Content from Specific UV Absorption. Croué et al. (2) have compiled percent aromatic C content (% C_{Ar}) versus specific UV absorbance at 254 nm (SUVA₂₅₄, L/m ·mg OC) data from several sources and shown that a good predictive relationship ($R^2 = 0.65$) holds for a range of humic materials. Although an equation quantifying the relationship was not provided, we estimated the following model from the published figure (see Figure. 4-3 A in Croué et al.(2)):

$$\% C_{Ar} = 5.2 \text{ SUVA}_{254} + 0.7 \quad (1)$$

Determination of 8:2 FTOH Enhanced Solubility Equilibration Time. In preliminary experiments, excess 8:2 FTOH was added to centrifuge tubes as crystals rather than plating the compound onto the glass surface. High variation in the observed 8:2 FTOH solubility with the excess crystals method (see below) was initially attributed to insufficient equilibration time. An equilibration time of 6 days was chosen as it appeared to be a reasonable compromise between minimizing variation in solubility measurements and risking unwanted compound loss by degradation. However, later experiments showed that variation could be reduced by plating the 8:2 FTOH and that equilibrium was achieved in < 6 days (Figure SI-1). However, the 6 day equilibration period was maintained to ensure that conditions as close to equilibrium as possible were attained and because we did not observe significant 8:2 FTOH degradation over this time period.

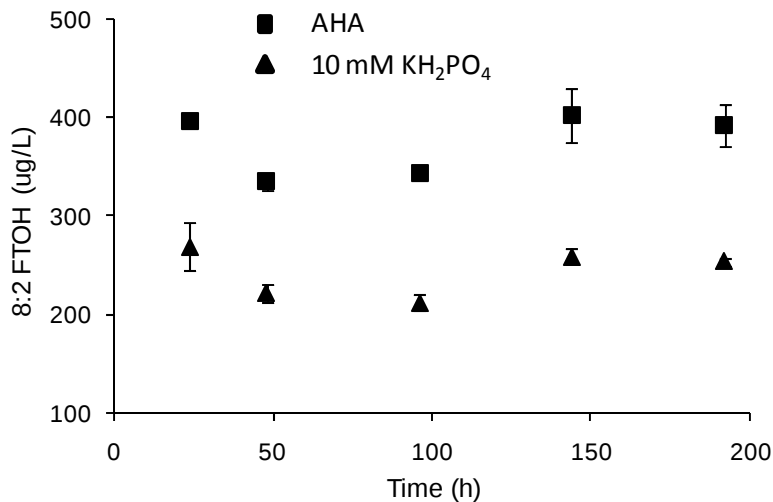


FIGURE SI-1. Solubility of 8:2 FTOH in 10 mM KH₂PO₄ (pH 7) and 145 mg OC/L AHA solution measured over 8 days.

Variation in 8:2 FTOH Solubility Measurements. Achieving consistent 8:2 FTOH concentration measurements in aqueous solutions proved to be challenging. Preliminary experiments conducted by adding excess 8:2 FTOH crystals to the tube reactors instead of plating the material onto the glass resulted in higher mean 8:2 FTOH concentrations and average coefficients of variation of 18% and 12% for replicates taken from a single centrifuge tube in experiments conducted with 7CB2 and AHA, respectively. Plating the 8:2 FTOH onto the tubes reduced this variation by approximately half to 8% for 7CB2 and 5% for AHA. Solubility measurements obtained with the excess crystal and plating techniques for 7CB2 are shown in Figure SI-2. Plating the 8:2 FTOH generated a thin film that became suspended in solution upon mixing. By comparison, the addition of crystals generated a suspension of particles with variable sizes and surface areas that may not have been fully separated from the aqueous phase prior to obtaining sample aliquots. This error could result in the positive bias observed for the excess crystal technique (3).

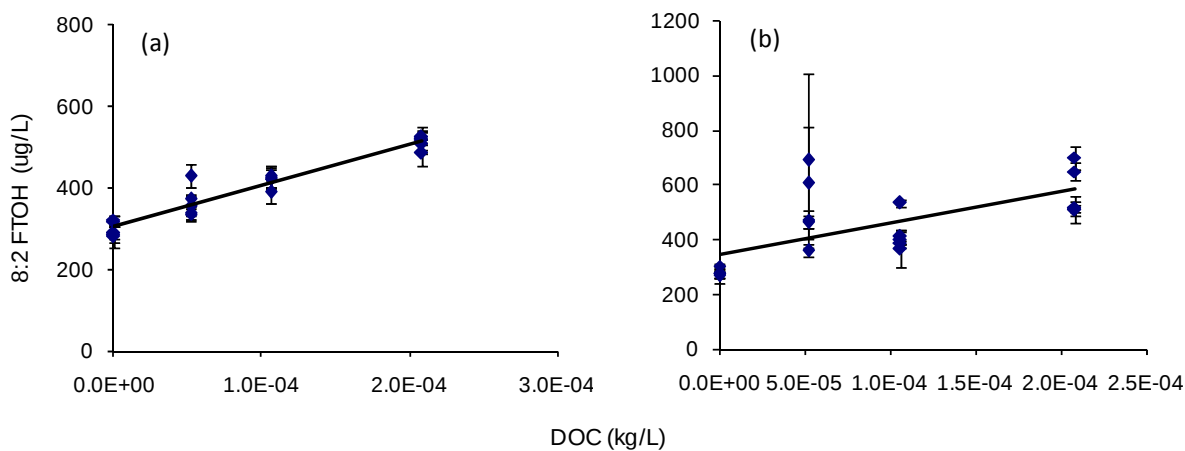


FIGURE SI-2. Comparison of variation observed for 8:2 FTOH enhanced solubility curves obtained by (a) plating excess compound on the glass centrifuge tubes and (b) adding excess loose crystals to the centrifuge tubes.

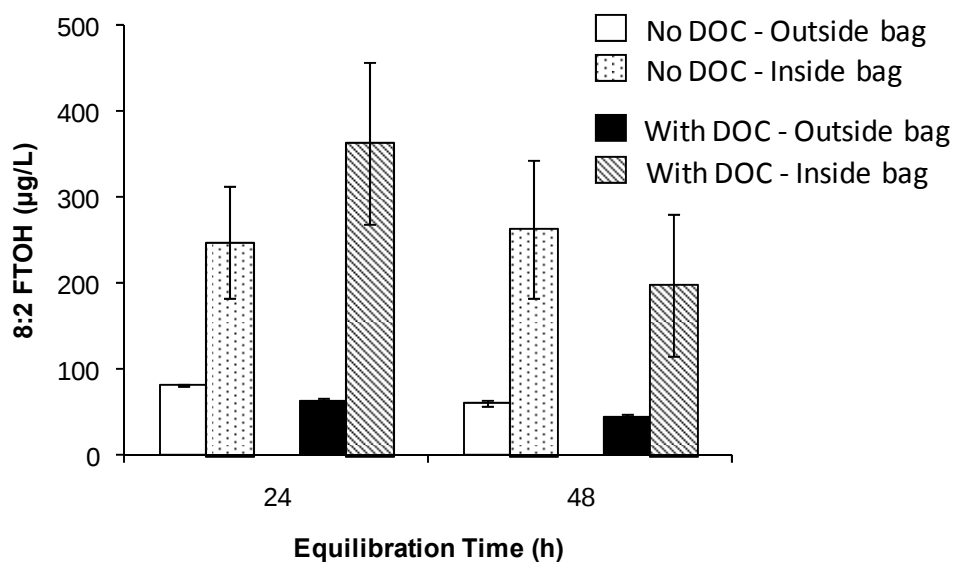


FIGURE SI-3. 8:2 FTOH concentrations measured inside and outside of dialysis bags in the presence and absence of DOC. Dialysis bags with DOC contained 154 mg OC/L as Aldrich humic acid prepared in 10 mM KH_2PO_4 at pH 7.0. Control dialysis bags were filled with 10 mM KH_2PO_4 at pH 7.0.

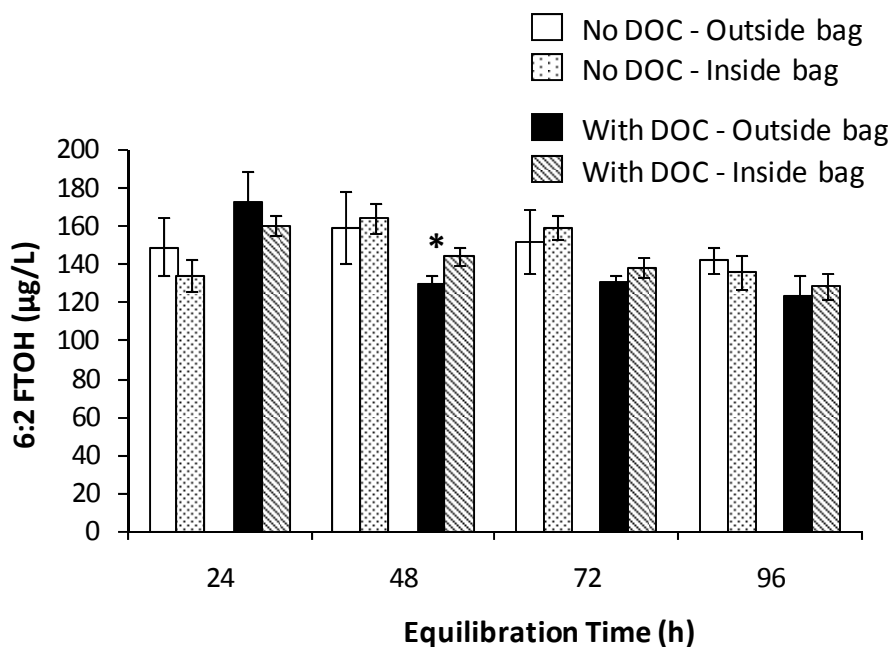


FIGURE SI-4. 6:2 FTOH concentrations measured inside and outside of dialysis bags in the presence and absence of DOC. Dialysis bags containing DOC at 900 mg OC/L as Aldrich humic acid prepared in 10 mM KH_2PO_4 at pH 7.0. Control dialysis bags were filled with 10 mM KH_2PO_4 at pH 7.0.

Effect of Salt Concentration on the Activity of 8:2 FTOH in Aqueous Solution. The effect of salt concentration on the activity of a compound in an aqueous solution is described by the relationship:

$$\frac{\gamma_{w,salt}}{\gamma_w} = 10^{K^s [\text{salt}]_{\text{tot}}} \quad (2)$$

where $\gamma_{iw,salt}$ and γ_{iw} are the compound's activity coefficients in the presence and absence of salt, respectively, K^s is the Setschenow or salting constant (M^{-1}), and $[\text{salt}]_{\text{tot}}$ is the total salt concentration in solution (M) (4). Studies conducted in seawater show that K^s values for diverse hydrophobic organic compounds range from 0.15 to $\sim 0.72 \text{ M}^{-1}$ (4). In our study, the LAF biosolids DOC matrix had the highest total salt concentration (0.04 M) and a composition similar to seawater. At this salt concentration, the ratio of 8:2 FTOH's activity would range from a

minimum of 1.01 to a maximum of 1.07. Thus, the maximum potential decrease in 8:2 FTOH solubility (1 to 7 %) would be similar to the range of experimental error (~5%) that was encountered.

Recalculation of K_{oc} Values from Liu and Lee (1). During the preparation of this current work, an error was noted in the calculation of $\log K_{oc}$ values obtained by direct aqueous measurements by Liu and Lee (1); however, the measured K_d (L/kg) values reported in Table 4 of Liu and Lee (1) are correct. The recalculated values using the %OC values reported in Table 1 and the K_d values reported in Table 4 of Liu and Lee (1) are listed in Table SI-1.

Table SI-1. Recalculated OC-Normalized Sorption Coefficients ($\log K_{oc}$) Values for Five Soils from Liu and Lee (1).	
Soil	$\log K_{oc}$
EPA-14	3.85
Drummer-6	3.77
Oakville-24	3.73
7CB2	3.74
SK961089	3.77
Average	3.77
Standard Deviation	0.05

Recalculation of Estimated K_{Leo} Values Using a Modified pp-LFER Paramter. We recalculated K_{Leo} values using the pp-LFER used by Goss et al. (5) combined with a modification to a parameter from Goss and Bronner (6). The pp-LFER first proposed by Niederer et al. (7) was developed by from a pp-LFER for Leonardite humic acid (LEO) (solid phase coated on glass beads)/air (98% relative humidity) and air/water partitioning information. Equation 3 in Niederer et al. (7) is the pp-LFER at 15°C, but the sorbent descriptors at other temperatures are provided in their Supporting Information. At 25°C the pp-LFER is:

$$\log K_{Leo} = 0.23 L_i + 2.52 V_i - 3.08 B_i - 0.49 A_i - 0.93 S_i + 0.27 \quad (4)$$

where V_i (100 cm³/mol) and L_i (m³/m³) are the McGowan molar volume and the logarithm of the hexadecane/air partition constant, respectively, which describe the compound's nonspecific interactions (i.e., cavity formation and van der Waals interactions). Note that in our current work we used the symbol K_{ha} is used instead of L_i to maintain a consistent format with other partition coefficients. B_i is the overall hydrogen-bond basicity (H-acceptor or electron-donor interactions), A_i is the overall hydrogen-bond acidity (H-donor or electron-acceptor interactions), and S_i is predominantly a description of electrostatic interaction established by dipole-dipole interactions but also incorporates some minor effects of polarizability.

Goss and Bronner (6) proposed a refinement to the L_i term to account for certain unique properties of PFCs, such as relatively weaker van der Waals interactions relative to hydrogenated counterparts. To more accurately capture the behavior of PFCs, they revised L_i according to the equation:

$$\log L_i = -0.022 V_i + 0.19 mr_i \quad (5)$$

where mr_i , the molar refraction of the compound, is reported in Arp et al. (8). We used this modification to L_i to recalculate K_{Leo} using eq. 4 above. Previously reported compound descriptors for 4:2 to 10:2 FTOH (8) are provided in Table SI-2, along with the modified L_i values we calculated with eqn. 5 that were used to recalculate K_{Leo} with eq. 4.

Table SI-2. Molar Refraction and Compound Descriptors for FTOHs from Goss et al. (5) and Arp et al. (8).

FTOH	mr_i	V_i (100 cm ³ /mol)	Original L_i (m ³ /m ³)	Modified L_i (m ³ /m ³)	A_i (SD)	B_i (SD)	S_i (SD)
4:2	0.2632	1.35	2.52	0.020	0.55 (0.04)	0.25 (0.04)	0.20 (0.07)
6:2	0.3481	1.78	2.96	0.027	0.55 (0.04)	0.25 (0.04)	0.20 (0.07)
8:2	0.4202	2.22	3.47	0.031	0.55 (0.04)	0.25 (0.04)	0.20 (0.07)
10:2	0.5107	2.65	3.9	0.039	0.55 (0.04)	0.25 (0.04)	0.20 (0.07)

Table SI-3. 8:2 FTOH Enhanced Solubility Measurements Raw Data. Bracketed and italicized values indicate the data point was excluded from the calculation of means. See the Methods and Materials for details on the criteria used to exclude data points.

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
LEO-HA ^a	0	1	1	244	273	22
LEO-HA	0	1	2	294		
LEO-HA	0	1	3	276		
LEO-HA	0	1	4	256		
LEO-HA	0	1	5	294		
LEO-HA	0	2	1	280	277	17
LEO-HA	0	2	2	254		
LEO-HA	0	2	3	296		
LEO-HA	0	2	4	(1530)		
LEO-HA	0	2	5	278		
LEO-HA	0	3	1	244	236	12
LEO-HA	0	3	2	234		
LEO-HA	0	3	3	228		
LEO-HA	0	3	4	224		
LEO-HA	0	3	5	252		
LEO-HA	0	4	1	234	242	11
LEO-HA	0	4	2	230		
LEO-HA	0	4	3	250		
LEO-HA	0	4	4	252		
LEO-HA	0	4	5	(454)		
LEO-HA	0	5	1	274	271	19
LEO-HA	0	5	2	(460)		
LEO-HA	0	5	3	296		
LEO-HA	0	5	4	258		
LEO-HA	0	5	5	256		
LEO-HA	25.6	1	1	360	344	12
LEO-HA	25.6	1	2	336		
LEO-HA	25.6	1	3	(4900)		
LEO-HA	25.6	1	4	334		
LEO-HA	25.6	1	5	344		
LEO-HA	25.6	2	1	294	282	12
LEO-HA	25.6	2	2	266		
LEO-HA	25.6	2	3	284		
LEO-HA	25.6	2	4	284		
LEO-HA	25.6	2	5	141		
LEO-HA	25.6	3	1	276	268	8
LEO-HA	25.6	3	2	274		
LEO-HA	25.6	3	3	262		
LEO-HA	25.6	3	4	268		
LEO-HA	25.6	3	5	258		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
LEO-HA	25.6	4	1	276	284	9
LEO-HA	25.6	4	2	290		
LEO-HA	25.6	4	3	282		
LEO-HA	25.6	4	4	296		
LEO-HA	25.6	4	5	276		
LEO-HA	25.6	5	1	342	326	19
LEO-HA	25.6	5	2	310		
LEO-HA	25.6	5	3	322		
LEO-HA	25.6	5	4	306		
LEO-HA	25.6	5	5	350		
LEO-HA	51.1	1	1	304	300	27
LEO-HA	51.1	1	2	328		
LEO-HA	51.1	1	3	318		
LEO-HA	51.1	1	4	292		
LEO-HA	51.1	1	5	258		
LEO-HA	51.1	2	1	314	321	17
LEO-HA	51.1	2	2	306		
LEO-HA	51.1	2	3	328		
LEO-HA	51.1	2	4	308		
LEO-HA	51.1	2	5	348		
LEO-HA	51.1	3	1	284	281	19
LEO-HA	51.1	3	2	258		
LEO-HA	51.1	3	3	310		
LEO-HA	51.1	3	4	278		
LEO-HA	51.1	3	5	274		
LEO-HA	51.1	4	1	270	268	7
LEO-HA	51.1	4	2	278		
LEO-HA	51.1	4	3	260		
LEO-HA	51.1	4	4	266		
LEO-HA	51.1	4	5	264		
LEO-HA	51.1	5	1	286	320	19
LEO-HA	51.1	5	2	330		
LEO-HA	51.1	5	3	328		
LEO-HA	51.1	5	4	326		
LEO-HA	51.1	5	5	328		
LEO-HA	102	1	1	322	310	37
LEO-HA	102	1	2	282		
LEO-HA	102	1	3	364		
LEO-HA	102	1	4	314		
LEO-HA	102	1	5	268		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
LEO-HA	102	2	1	368	393	15
LEO-HA	102	2	2	404		
LEO-HA	102	2	3	390		
LEO-HA	102	2	4	398		
LEO-HA	102	2	5	404		
LEO-HA	102	3	1	338	325	15
LEO-HA	102	3	2	304		
LEO-HA	102	3	3	340		
LEO-HA	102	3	4	326		
LEO-HA	102	3	5	318		
LEO-HA	102	4	1	360	384	26
LEO-HA	102	4	2	360		
LEO-HA	102	4	3	376		
LEO-HA	102	4	4	410		
LEO-HA	102	4	5	412		
LEO-HA	102	5	1	348	336	29
LEO-HA	102	5	2	312		
LEO-HA	102	5	3	362		
LEO-HA	102	5	4	358		
LEO-HA	102	5	5	298		
LEO-HA	205	1	1	482	451	19
LEO-HA	205	1	2	450		
LEO-HA	205	1	3	446		
LEO-HA	205	1	4	446		
LEO-HA	205	1	5	432		
LEO-HA	205	2	1	442	428	17
LEO-HA	205	2	2	428		
LEO-HA	205	2	3	446		
LEO-HA	205	2	4	418		
LEO-HA	205	2	5	404		
LEO-HA	205	3	1	434	431	11
LEO-HA	205	3	2	446		
LEO-HA	205	3	3	434		
LEO-HA	205	3	4	422		
LEO-HA	205	3	5	420		
LEO-HA	205	4	1	490	447	25
LEO-HA	205	4	2	442		
LEO-HA	205	4	3	432		
LEO-HA	205	4	4	432		
LEO-HA	205	4	5	438		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
LEO-HA	205	5	1	440	488	35
LEO-HA	205	5	2	484		
LEO-HA	205	5	3	530		
LEO-HA	205	5	4	476		
LEO-HA	205	5	5	512		
AHA ^b	0	1	1	296	280	25
AHA	0	1	2	314		
AHA	0	1	3	274		
AHA	0	1	4	254		
AHA	0	1	5	262		
AHA	0	2	1	310	288	21
AHA	0	2	2	284		
AHA	0	2	3	286		
AHA	0	2	4	302		
AHA	0	2	5	256		
AHA	0	3	1	332	318	13
AHA	0	3	2	326		
AHA	0	3	3	320		
AHA	0	3	4	298		
AHA	0	3	5	316		
AHA	0	4	1	320	322	11
AHA	0	4	2	340		
AHA	0	4	3	320		
AHA	0	4	4	320		
AHA	0	4	5	310		
AHA	0	5	1	288	290	15
AHA	0	5	2	268		
AHA	0	5	3	310		
AHA	0	5	4	292		
AHA	0	5	5	290		
AHA	52.2	1	1	328	336	18
AHA	52.2	1	2	322		
AHA	52.2	1	3	334		
AHA	52.2	1	4	366		
AHA	52.2	1	5	328		
AHA	52.2	2	1	378	356	22
AHA	52.2	2	2	366		
AHA	52.2	2	3	352		
AHA	52.2	2	4	326		
AHA	52.2	2	5	(732)		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
AHA	52.2	3	1	376	372	13
AHA	52.2	3	2	374		
AHA	52.2	3	3	386		
AHA	52.2	3	4	372		
AHA	52.2	3	5	350		
AHA	52.2	4	1	524	(474.4)	36
AHA	52.2	4	2	424		
AHA	52.2	4	3	486		
AHA	52.2	4	4	470		
AHA	52.2	4	5	468		
AHA	52.2	5	1	332	336	13
AHA	52.2	5	2	318		
AHA	52.2	5	3	346		
AHA	52.2	5	4	334		
AHA	52.2	5	5	352		
AHA	106.23	1	1	450	428	26
AHA	106.23	1	2	454		
AHA	106.23	1	3	390		
AHA	106.23	1	4	428		
AHA	106.23	1	5	416		
AHA	106.23	2	1	402	410	34
AHA	106.23	2	2	422		
AHA	106.23	2	3	458		
AHA	106.23	2	4	406		
AHA	106.23	2	5	364		
AHA	106.23	3	1	454	422	22
AHA	106.23	3	2	406		
AHA	106.23	3	3	416		
AHA	106.23	3	4	434		
AHA	106.23	3	5	400		
AHA	106.23	4	1	428	418	10
AHA	106.23	4	2	426		
AHA	106.23	4	3	410		
AHA	106.23	4	4	408		
AHA	106.23	4	5	(474)		
AHA	106.23	5	1	394	391	28
AHA	106.23	5	2	402		
AHA	106.23	5	3	428		
AHA	106.23	5	4	354		
AHA	106.23	5	5	376		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
AHA	208.05	1	1	492	506	13
AHA	208.05	1	2	510		
AHA	208.05	1	3	494		
AHA	208.05	1	4	520		
AHA	208.05	1	5	516		
AHA	208.05	2	1	516	523	15
AHA	208.05	2	2	548		
AHA	208.05	2	3	510		
AHA	208.05	2	4	520		
AHA	208.05	2	5	520		
AHA	208.05	3	1	528	524	14
AHA	208.05	3	2	544		
AHA	208.05	3	3	522		
AHA	208.05	3	4	524		
AHA	208.05	3	5	504		
AHA	208.05	4	1	528	519	32
AHA	208.05	4	2	570		
AHA	208.05	4	3	498		
AHA	208.05	4	4	510		
AHA	208.05	4	5	488		
AHA	208.05	5	1	538	486	34
AHA	208.05	5	2	480		
AHA	208.05	5	3	470		
AHA	208.05	5	4	496		
AHA	208.05	5	5	448		
PP-HA ^c	0	1	1	300	285	11
PP-HA	0	1	2	284		
PP-HA	0	1	3	272		
PP-HA	0	1	4	290		
PP-HA	0	1	5	280		
PP-HA	0	2	1	290	283	18
PP-HA	0	2	2	278		
PP-HA	0	2	3	274		
PP-HA	0	2	4	264		
PP-HA	0	2	5	310		
PP-HA	0	3	1	306	304	16
PP-HA	0	3	2	300		
PP-HA	0	3	3	314		
PP-HA	0	3	4	278		
PP-HA	0	3	5	320		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
PP-HA	0	4	1	298	288	17
PP-HA	0	4	2	290		
PP-HA	0	4	3	306		
PP-HA	0	4	4	282		
PP-HA	0	4	5	262		
PP-HA	0	5	1	258	265	11
PP-HA	0	5	2	280		
PP-HA	0	5	3	254		
PP-HA	0	5	4	274		
PP-HA	0	5	5	258		
PP-HA	48.45	1	1	334	337	23
PP-HA	48.45	1	2	360		
PP-HA	48.45	1	3	330		
PP-HA	48.45	1	4	304		
PP-HA	48.45	1	5	356		
PP-HA	48.45	2	1	354	332	15
PP-HA	48.45	2	2	336		
PP-HA	48.45	2	3	328		
PP-HA	48.45	2	4	330		
PP-HA	48.45	2	5	314		
PP-HA	48.45	3	1	358	342	13
PP-HA	48.45	3	2	350		
PP-HA	48.45	3	3	346		
PP-HA	48.45	3	4	326		
PP-HA	48.45	3	5	332		
PP-HA	48.45	4	1	366	361	8
PP-HA	48.45	4	2	358		
PP-HA	48.45	4	3	370		
PP-HA	48.45	4	4	362		
PP-HA	48.45	4	5	350		
PP-HA	48.45	5	1	334	333	11
PP-HA	48.45	5	2	340		
PP-HA	48.45	5	3	336		
PP-HA	48.45	5	4	314		
PP-HA	48.45	5	5	340		
PP-HA	95.92	1	1	398	379	15
PP-HA	95.92	1	2	384		
PP-HA	95.92	1	3	380		
PP-HA	95.92	1	4	358		
PP-HA	95.92	1	5	374		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
PP-HA	95.92	2	1	390	383	17
PP-HA	95.92	2	2	398		
PP-HA	95.92	2	3	358		
PP-HA	95.92	2	4	396		
PP-HA	95.92	2	5	374		
PP-HA	95.92	3	1	418	394	15
PP-HA	95.92	3	2	380		
PP-HA	95.92	3	3	394		
PP-HA	95.92	3	4	396		
PP-HA	95.92	3	5	384		
PP-HA	95.92	4	1	362	363	11
PP-HA	95.92	4	2	366		
PP-HA	95.92	4	3	376		
PP-HA	95.92	4	4	364		
PP-HA	95.92	4	5	346		
PP-HA	95.92	5	1	384	405	15
PP-HA	95.92	5	2	410		
PP-HA	95.92	5	3	422		
PP-HA	95.92	5	4	398		
PP-HA	95.92	5	5	412		
PP-HA	195.47	1	1	432	414	21
PP-HA	195.47	1	2	402		
PP-HA	195.47	1	3	430		
PP-HA	195.47	1	4	384		
PP-HA	195.47	1	5	422		
PP-HA	195.47	2	1	498	489	10
PP-HA	195.47	2	2	500		
PP-HA	195.47	2	3	476		
PP-HA	195.47	2	4	490		
PP-HA	195.47	2	5	482		
PP-HA	195.47	3	1	436	445	9
PP-HA	195.47	3	2	458		
PP-HA	195.47	3	3	442		
PP-HA	195.47	3	4	438		
PP-HA	195.47	3	5	452		
PP-HA	195.47	4	1	466	462	11
PP-HA	195.47	4	2	474		
PP-HA	195.47	4	3	468		
PP-HA	195.47	4	4	446		
PP-HA	195.47	4	5	458		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
PP-HA	195.47	5	1	480	460	19
PP-HA	195.47	5	2	442		
PP-HA	195.47	5	3	472		
PP-HA	195.47	5	4	458		
PP-HA	195.47	5	5	na		
SK961089 ^d	0	1	1	256	256	4
SK961089	0	1	2	260		
SK961089	0	1	3	258		
SK961089	0	1	4	250		
SK961089	0	1	5	(330)		
SK961089	0	2	1	254	257	5
SK961089	0	2	2	258		
SK961089	0	2	3	252		
SK961089	0	2	4	266		
SK961089	0	2	5	256		
SK961089	0	3	1	248	269	18
SK961089	0	3	2	260		
SK961089	0	3	3	282		
SK961089	0	3	4	286		
SK961089	0	3	5	(336)		
SK961089	0	4	1	262	283	24
SK961089	0	4	2	258		
SK961089	0	4	3	282		
SK961089	0	4	4	312		
SK961089	0	4	5	302		
SK961089	0	5	1	252	274	24
SK961089	0	5	2	252		
SK961089	0	5	3	284		
SK961089	0	5	4	270		
SK961089	0	5	5	310		
SK961089	14	1	1	284	302	16
SK961089	14	1	2	288		
SK961089	14	1	3	310		
SK961089	14	1	4	308		
SK961089	14	1	5	322		
SK961089	14	2	1	280	285	7
SK961089	14	2	2	280		
SK961089	14	2	3	296		
SK961089	14	2	4	282		
SK961089	14	2	5	286		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
SK961089	14	3	1	318	318	9
SK961089	14	3	2	314		
SK961089	14	3	3	328		
SK961089	14	3	4	306		
SK961089	14	3	5	326		
SK961089	14	4	1	316	297	13
SK961089	14	4	2	288		
SK961089	14	4	3	304		
SK961089	14	4	4	284		
SK961089	14	4	5	294		
SK961089	14	5	1	296	301	17
SK961089	14	5	2	290		
SK961089	14	5	3	330		
SK961089	14	5	4	290		
SK961089	14	5	5	298		
SK961089	27	1	1	322	(420)	110
SK961089	27	1	2	386		
SK961089	27	1	3	358		
SK961089	27	1	4	436		
SK961089	27	1	5	602		
SK961089	27	2	1	326	322	8
SK961089	27	2	2	314		
SK961089	27	2	3	330		
SK961089	27	2	4	328		
SK961089	27	2	5	314		
SK961089	27	3	1	336	330	13
SK961089	27	3	2	322		
SK961089	27	3	3	326		
SK961089	27	3	4	316		
SK961089	27	3	5	348		
SK961089	27	4	1	322	332	9
SK961089	27	4	2	342		
SK961089	27	4	3	342		
SK961089	27	4	4	326		
SK961089	27	4	5	328		
SK961089	27	5	1	326	321	6
SK961089	27	5	2	328		
SK961089	27	5	3	322		
SK961089	27	5	4	312		
SK961089	27	5	5	318		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
SK961089	54	1	1	358	393	30
SK961089	54	1	2	(470)		
SK961089	54	1	3	424		
SK961089	54	1	4	410		
SK961089	54	1	5	378		
SK961089	54	2	1	386	392	12
SK961089	54	2	2	410		
SK961089	54	2	3	390		
SK961089	54	2	4	(560)		
SK961089	54	2	5	382		
SK961089	54	3	1	394	392	9
SK961089	54	3	2	390		
SK961089	54	3	3	406		
SK961089	54	3	4	382		
SK961089	54	3	5	390		
SK961089	54	4	1	398	388	9
SK961089	54	4	2	394		
SK961089	54	4	3	388		
SK961089	54	4	4	384		
SK961089	54	4	5	374		
SK961089	54	5	1	394	395	6
SK961089	54	5	2	400		
SK961089	54	5	3	390		
SK961089	54	5	4	388		
SK961089	54	5	5	402		
SK961089	108	1	1	528	528	7
SK961089	108	1	2	520		
SK961089	108	1	3	534		
SK961089	108	1	4	534		
SK961089	108	1	5	522		
SK961089	108	2	1	558	536	17
SK961089	108	2	2	550		
SK961089	108	2	3	530		
SK961089	108	2	4	520		
SK961089	108	2	5	524		
SK961089	108	3	1	506	519	15
SK961089	108	3	2	530		
SK961089	108	3	3	536		
SK961089	108	3	4	520		
SK961089	108	3	5	502		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
SK961089	108	4	1	524	524	14
SK961089	108	4	2	524		
SK961089	108	4	3	540		
SK961089	108	4	4	528		
SK961089	108	4	5	502		
SK961089	108	5	1	576	566	17
SK961089	108	5	2	550		
SK961089	108	5	3	590		
SK961089	108	5	4	558		
SK961089	108	5	5	556		
7CB2 ^e	0	1	1	278	283	6
7CB2	0	1	2	286		
7CB2	0	1	3	284		
7CB2	0	1	4	276		
7CB2	0	1	5	290		
7CB2	0	2	1	290	294	10
7CB2	0	2	2	288		
7CB2	0	2	3	288		
7CB2	0	2	4	294		
7CB2	0	2	5	312		
7CB2	0	3	1	294	278	15
7CB2	0	3	2	276		
7CB2	0	3	3	286		
7CB2	0	3	4	282		
7CB2	0	3	5	254		
7CB2	0	4	1	274	257	12
7CB2	0	4	2	242		
7CB2	0	4	3	250		
7CB2	0	4	4	262		
7CB2	0	4	5	258		
7CB2	0	5	1	288	280	9
7CB2	0	5	2	280		
7CB2	0	5	3	264		
7CB2	0	5	4	284		
7CB2	0	5	5	284		
7CB2	24.907	1	1	308	294	13
7CB2	24.907	1	2	294		
7CB2	24.907	1	3	278		
7CB2	24.907	1	4	284		
7CB2	24.907	1	5	306		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
7CB2	24.907	2	1	274	275	12
7CB2	24.907	2	2	292		
7CB2	24.907	2	3	272		
7CB2	24.907	2	4	262		
7CB2	24.907	2	5	(332)		
7CB2	24.907	3	1	280	287	6
7CB2	24.907	3	2	292		
7CB2	24.907	3	3	(332)		
7CB2	24.907	3	4	284		
7CB2	24.907	3	5	290		
7CB2	24.907	4	1	293	284	7
7CB2	24.907	4	2	291		
7CB2	24.907	4	3	282		
7CB2	24.907	4	4	276		
7CB2	24.907	4	5	279		
7CB2	24.907	5	1	286	280	18
7CB2	24.907	5	2	274		
7CB2	24.907	5	3	252		
7CB2	24.907	5	4	298		
7CB2	24.907	5	5	290		
7CB2	49.45	1	1	304	307	27
7CB2	49.45	1	2	276		
7CB2	49.45	1	3	340		
7CB2	49.45	1	4	286		
7CB2	49.45	1	5	328		
7CB2	49.45	2	1	284	288	5
7CB2	49.45	2	2	288		
7CB2	49.45	2	3	294		
7CB2	49.45	2	4	284		
7CB2	49.45	2	5	(330)		
7CB2	49.45	3	1	276	270	17
7CB2	49.45	3	2	290		
7CB2	49.45	3	3	270		
7CB2	49.45	3	4	270		
7CB2	49.45	3	5	242		
7CB2	49.45	4	1	318	316	6
7CB2	49.45	4	2	306		
7CB2	49.45	4	3	316		
7CB2	49.45	4	4	320		
7CB2	49.45	4	5	318		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
7CB2	49.45	5	1	334	(674)	546
7CB2	49.45	5	2	282		
7CB2	49.45	5	3	1600		
7CB2	49.45	5	4	426		
7CB2	49.45	5	5	728		
7CB2	100.51	1	1	280	290	8
7CB2	100.51	1	2	300		
7CB2	100.51	1	3	290		
7CB2	100.51	1	4	294		
7CB2	100.51	1	5	284		
7CB2	100.51	2	1	298	304	13
7CB2	100.51	2	2	304		
7CB2	100.51	2	3	302		
7CB2	100.51	2	4	290		
7CB2	100.51	2	5	326		
7CB2	100.51	3	1	314	334	17
7CB2	100.51	3	2	336		
7CB2	100.51	3	3	320		
7CB2	100.51	3	4	344		
7CB2	100.51	3	5	356		
7CB2	100.51	4	1	320	348	39
7CB2	100.51	4	2	314		
7CB2	100.51	4	3	332		
7CB2	100.51	4	4	364		
7CB2	100.51	4	5	408		
7CB2	100.51	5	1	324	314	15
7CB2	100.51	5	2	300		
7CB2	100.51	5	3	296		
7CB2	100.51	5	4	324		
7CB2	100.51	5	5	326		
LAF ^f	0	1	1	248	256	13
LAF	0	1	2	274		
LAF	0	1	3	258		
LAF	0	1	4	240		
LAF	0	1	5	258		
LAF	0	2	1	278	267	9
LAF	0	2	2	276		
LAF	0	2	3	262		
LAF	0	2	4	264		
LAF	0	2	5	256		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
LAF	0	3	1	248	253	4
LAF	0	3	2	256		
LAF	0	3	3	250		
LAF	0	3	4	258		
LAF	0	3	5	252		
LAF	0	4	1	(356)	273	13
LAF	0	4	2	290		
LAF	0	4	3	260		
LAF	0	4	4	272		
LAF	0	4	5	268		
LAF	0	5	1	284	255	22
LAF	0	5	2	242		
LAF	0	5	3	272		
LAF	0	5	4	244		
LAF	0	5	5	234		
LAF	23.93	1	1	300	292	11
LAF	23.93	1	2	296		
LAF	23.93	1	3	278		
LAF	23.93	1	4	304		
LAF	23.93	1	5	282		
LAF	23.93	2	1	282	271	10
LAF	23.93	2	2	264		
LAF	23.93	2	3	282		
LAF	23.93	2	4	262		
LAF	23.93	2	5	266		
LAF	23.93	3	1	272	268	11
LAF	23.93	3	2	270		
LAF	23.93	3	3	270		
LAF	23.93	3	4	278		
LAF	23.93	3	5	250		
LAF	23.93	4	1	266	266	13
LAF	23.93	4	2	286		
LAF	23.93	4	3	266		
LAF	23.93	4	4	256		
LAF	23.93	4	5	254		
LAF	23.93	5	1	296	275	15
LAF	23.93	5	2	274		
LAF	23.93	5	3	260		
LAF	23.93	5	4	282		
LAF	23.93	5	5	262		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
LAF	47.86	1	1	312	289	15
LAF	47.86	1	2	282		
LAF	47.86	1	3	278		
LAF	47.86	1	4	294		
LAF	47.86	1	5	278		
LAF	47.86	2	1	300	293	15
LAF	47.86	2	2	286		
LAF	47.86	2	3	316		
LAF	47.86	2	4	278		
LAF	47.86	2	5	286		
LAF	47.86	3	1	294	266	21
LAF	47.86	3	2	282		
LAF	47.86	3	3	248		
LAF	47.86	3	4	254		
LAF	47.86	3	5	250		
LAF	47.86	4	1	292	286	9
LAF	47.86	4	2	296		
LAF	47.86	4	3	288		
LAF	47.86	4	4	276		
LAF	47.86	4	5	278		
LAF	47.86	5	1	306	290	19
LAF	47.86	5	2	314		
LAF	47.86	5	3	278		
LAF	47.86	5	4	274		
LAF	47.86	5	5	278		
LAF	95.72	1	1	302	308	9
LAF	95.72	1	2	316		
LAF	95.72	1	3	320		
LAF	95.72	1	4	300		
LAF	95.72	1	5	304		
LAF	95.72	2	1	304	299	14
LAF	95.72	2	2	298		
LAF	95.72	2	3	312		
LAF	95.72	2	4	276		
LAF	95.72	2	5	304		
LAF	95.72	3	1	(354)	307	4
LAF	95.72	3	2	308		
LAF	95.72	3	3	308		
LAF	95.72	3	4	300		
LAF	95.72	3	5	310		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
LAF	95.72	4	1	310	328	13
LAF	95.72	4	2	334		
LAF	95.72	4	3	338		
LAF	95.72	4	4	320		
LAF	95.72	4	5	340		
LAF	95.72	5	1	330	319	9
LAF	95.72	5	2	314		
LAF	95.72	5	3	326		
LAF	95.72	5	4	312		
LAF	95.72	5	5	312		
WLAF ^g	0	1	1	270	269	7
WLAF	0	1	2	272		
WLAF	0	1	3	264		
WLAF	0	1	4	278		
WLAF	0	1	5	260		
WLAF	0	2	1	272	262	13
WLAF	0	2	2	258		
WLAF	0	2	3	270		
WLAF	0	2	4	240		
WLAF	0	2	5	268		
WLAF	0	3	1	(448)	249	9
WLAF	0	3	2	252		
WLAF	0	3	3	260		
WLAF	0	3	4	244		
WLAF	0	3	5	240		
WLAF	0	4	1	274	268	13
WLAF	0	4	2	272		
WLAF	0	4	3	258		
WLAF	0	4	4	284		
WLAF	0	4	5	252		
WLAF	0	5	1	280	277	5
WLAF	0	5	2	276		
WLAF	0	5	3	282		
WLAF	0	5	4	270		
WLAF	0	5	5	276		
WLAF	17.225	1	1	302	319	13
WLAF	17.225	1	2	324		
WLAF	17.225	1	3	312		
WLAF	17.225	1	4	320		
WLAF	17.225	1	5	336		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
WLAF	17.225	2	1	298	293	5
WLAF	17.225	2	2	286		
WLAF	17.225	2	3	296		
WLAF	17.225	2	4	292		
WLAF	17.225	2	5	(338)		
WLAF	17.225	3	1	270	267	4
WLAF	17.225	3	2	272		
WLAF	17.225	3	3	262		
WLAF	17.225	3	4	266		
WLAF	17.225	3	5	264		
WLAF	17.225	4	1	302	295	12
WLAF	17.225	4	2	298		
WLAF	17.225	4	3	288		
WLAF	17.225	4	4	278		
WLAF	17.225	4	5	308		
WLAF	17.225	5	1	296	290	11
WLAF	17.225	5	2	272		
WLAF	17.225	5	3	298		
WLAF	17.225	5	4	288		
WLAF	17.225	5	5	296		
WLAF	34.45	1	1	270	288	12
WLAF	34.45	1	2	296		
WLAF	34.45	1	3	282		
WLAF	34.45	1	4	302		
WLAF	34.45	1	5	288		
WLAF	34.45	2	1	(326)	290	4
WLAF	34.45	2	2	286		
WLAF	34.45	2	3	294		
WLAF	34.45	2	4	286		
WLAF	34.45	2	5	292		
WLAF	34.45	3	1	282	281	13
WLAF	34.45	3	2	272		
WLAF	34.45	3	3	270		
WLAF	34.45	3	4	278		
WLAF	34.45	3	5	302		
WLAF	34.45	4	1	304	292	9
WLAF	34.45	4	2	300		
WLAF	34.45	4	3	282		
WLAF	34.45	4	4	286		
WLAF	34.45	4	5	290		

DOC Source	DOC (mg/L)	Tube No.	Aliquot	8:2 FTOH (ug/L)	Average	Standard Deviation
WLAF	34.45	5	1	294	279	13
WLAF	34.45	5	2	280		
WLAF	34.45	5	3	290		
WLAF	34.45	5	4	270		
WLAF	34.45	5	5	262		
WLAF	68.9	1	1	266	280	15
WLAF	68.9	1	2	(342)		
WLAF	68.9	1	3	274		
WLAF	68.9	1	4	300		
WLAF	68.9	1	5	278		
WLAF	68.9	2	1	324	302	20
WLAF	68.9	2	2	282		
WLAF	68.9	2	3	280		
WLAF	68.9	2	4	310		
WLAF	68.9	2	5	314		
WLAF	68.9	3	1	288	298	11
WLAF	68.9	3	2	294		
WLAF	68.9	3	3	316		
WLAF	68.9	3	4	294		
WLAF	68.9	3	5	298		
WLAF	68.9	4	1	338	328	11
WLAF	68.9	4	2	322		
WLAF	68.9	4	3	314		
WLAF	68.9	4	4	328		
WLAF	68.9	4	5	340		
WLAF	68.9	5	1	292	282	11
WLAF	68.9	5	2	280		
WLAF	68.9	5	3	288		
WLAF	68.9	5	4	284		
WLAF	68.9	5	5	264		

^a Leonardite humic acid, ^b Aldrich humic acid, ^c Pahokee Peat humic acid, ^d SK961089 soil, ^e 7CB2 soil, ^f Lafayette biosolids, ^g West Lafayette biosolids.

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