Supplemental Information to

Experimental determination of the partitioning of representative organic pollutants to the air-water interface

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Figure S1. Bulk fluorescence vs. concentration plots for a) fluoranthene, b) pyrene, c) umbelliferone, d) phenol red e) BPA and f) naphthalene.

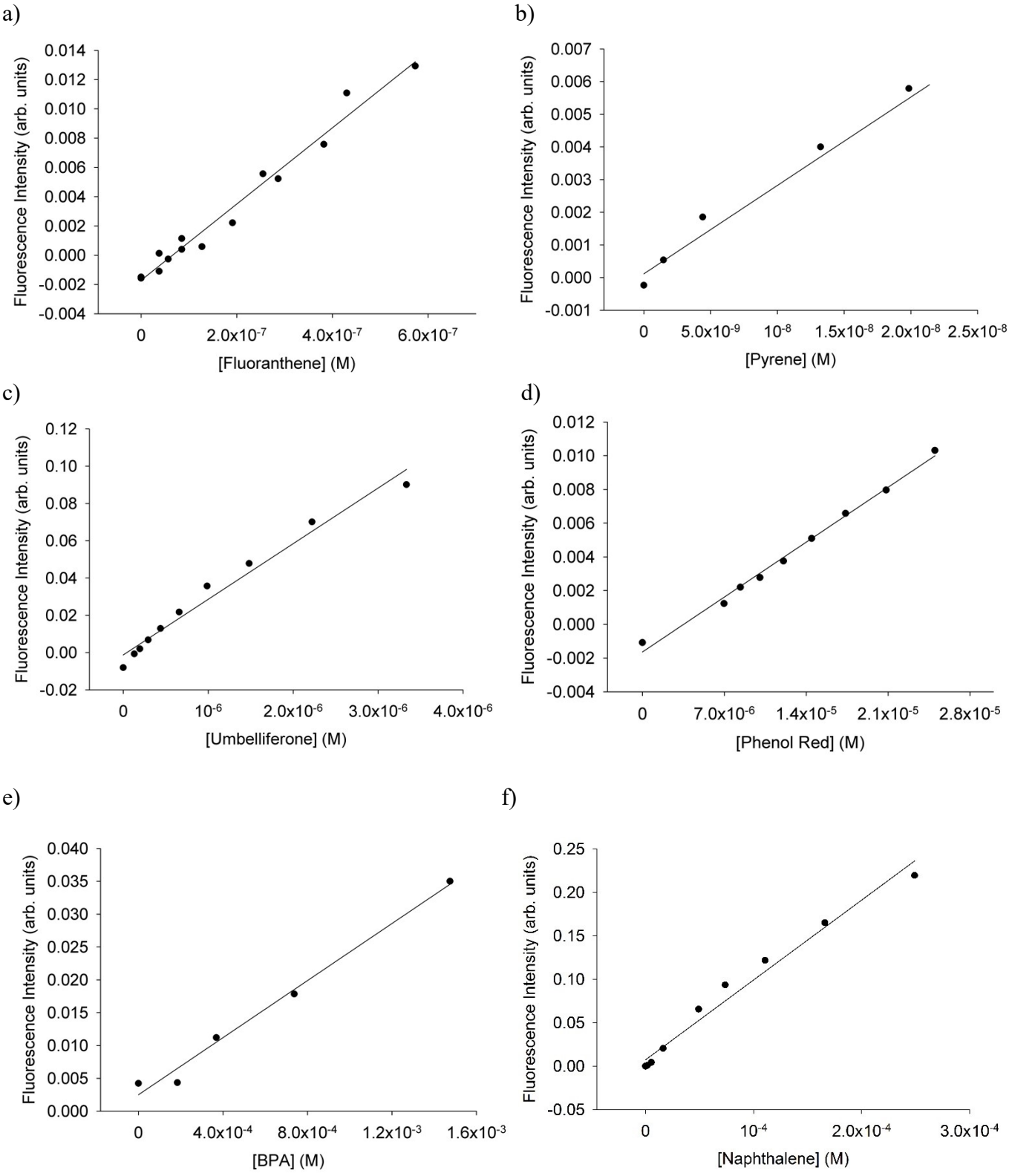


Figure S2. Absorption spectrum obtained from a PerkinElmer LAMBDA 365 double-beam UV-Vis spectrometer for saturated BPA in a 1 cm pathlength quartz cuvette taken immediately after filtration and cooling to room temperature. The concentration was calculated assuming a molar absorptivity coefficient of 14.86 cm^{-1} M^{-1} at 214 nm.[1]

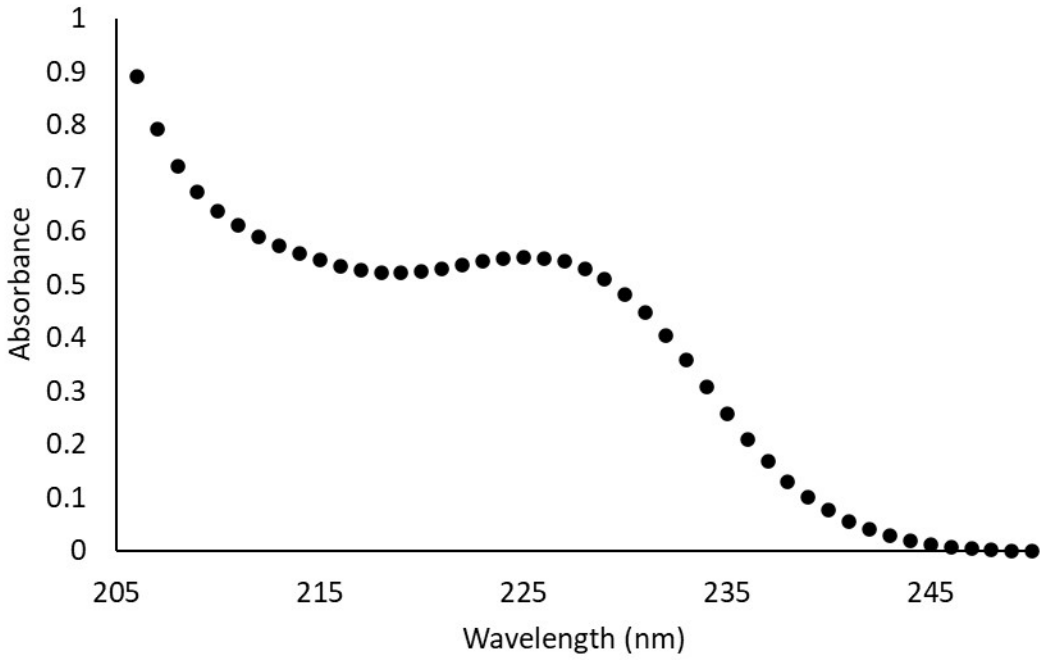
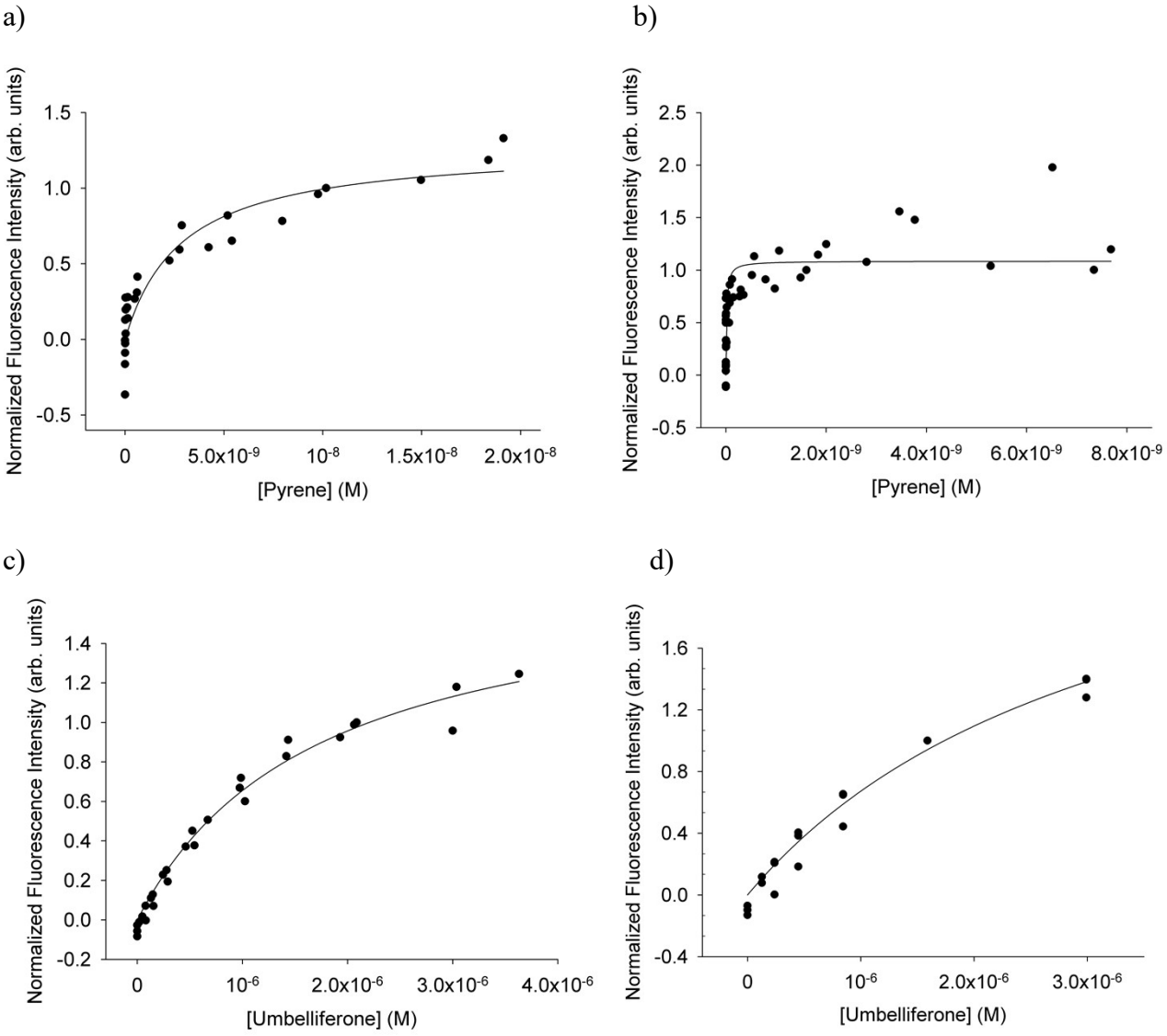
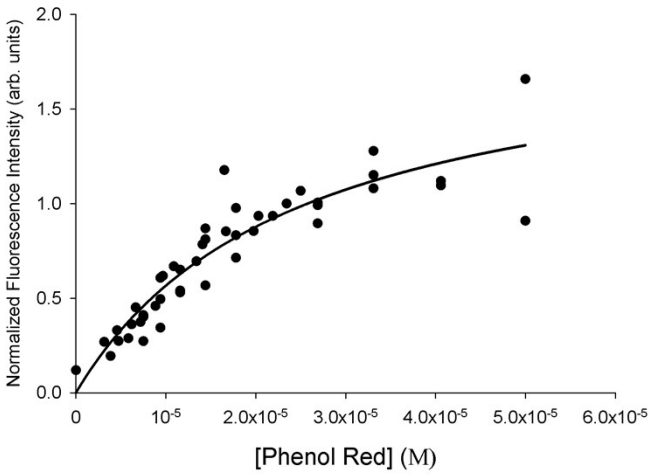


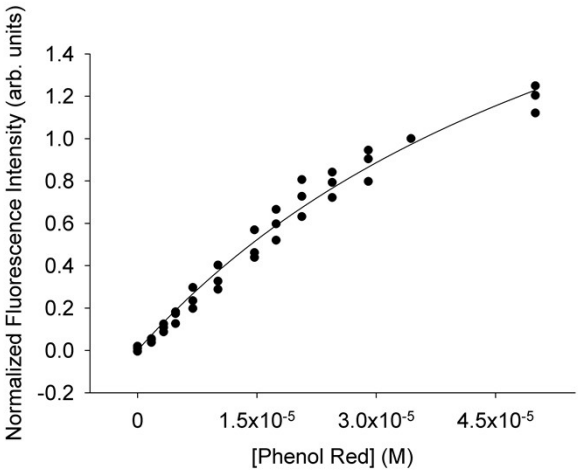
Figure S3. Langmuir isotherms for a) pyrene with a freshwater surface, b) pyrene with an octanol-coated surface, c) umbelliferone with a freshwater surface, d) umbelliferone with an octanol-coated surface, e) phenol red with a freshwater surface, f) phenol red with an octanol-coated surface, g) BPA with a freshwater surface, h) anthracene with a freshwater surface, i) IC with a freshwater surface,j) IC with an octanol-coated surface, k) naphthalene with a freshwater surface, and l) naphthalene with an octanol-coated surface.



e)


Normalized Fluorescence Intensity (arb. units)
2.0
1.5
1.0
0.5
0.0
0
10-5
2.0x10-5
3.0x10-5
4.0x10-5
5.0x10-5
6.0x10-5
[Phenol Red] (M)

f)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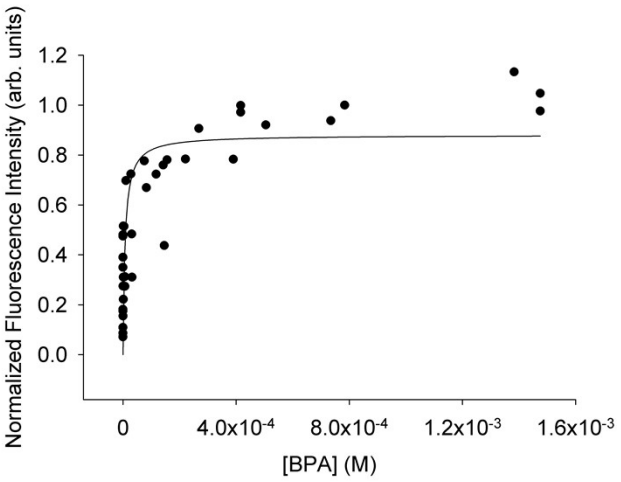
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
0
1.5x10-5
3.0x10-5
4.5x10-5
[Phenol Red] (M)

g)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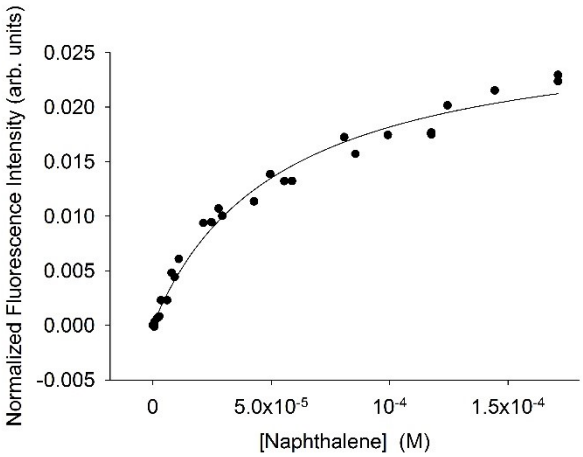
0.8
0.6
0.4
0.2
0.0
0
4.0x10-4
8.0x10-4
1.2x10-3
1.6x10-3
[BPA] (M)

k)


Normalized Fluorescence Intensity (arb. units)
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0.020
0.015
0.010
0.005
0.000
-0.005
0
5.0x10-5
10-4
1.5x10-4
[Naphthalene] (M)

l)

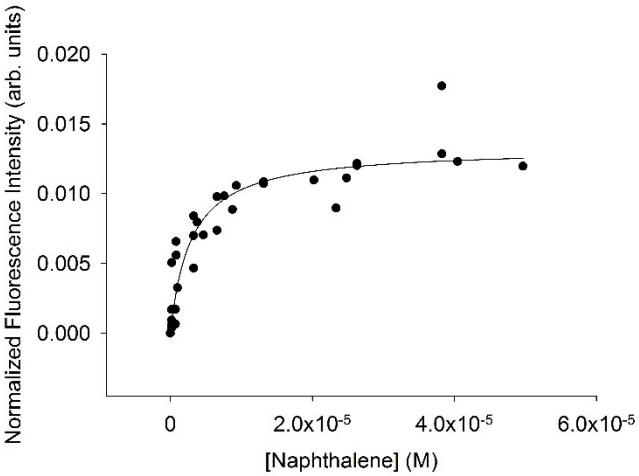
Normalized Fluorescence Intensity (arb. units)
0.020
0.015
0.010
0.005
0.000
0
2.0x10-5
4.0x10-5
6.0x10-5
[Naphthalene] (M)

Figure S4. Langmuir isotherms for a) anthracene with a freshwater surface, b) IC with a freshwater surface, and c) IC with an octanol-coated surface.

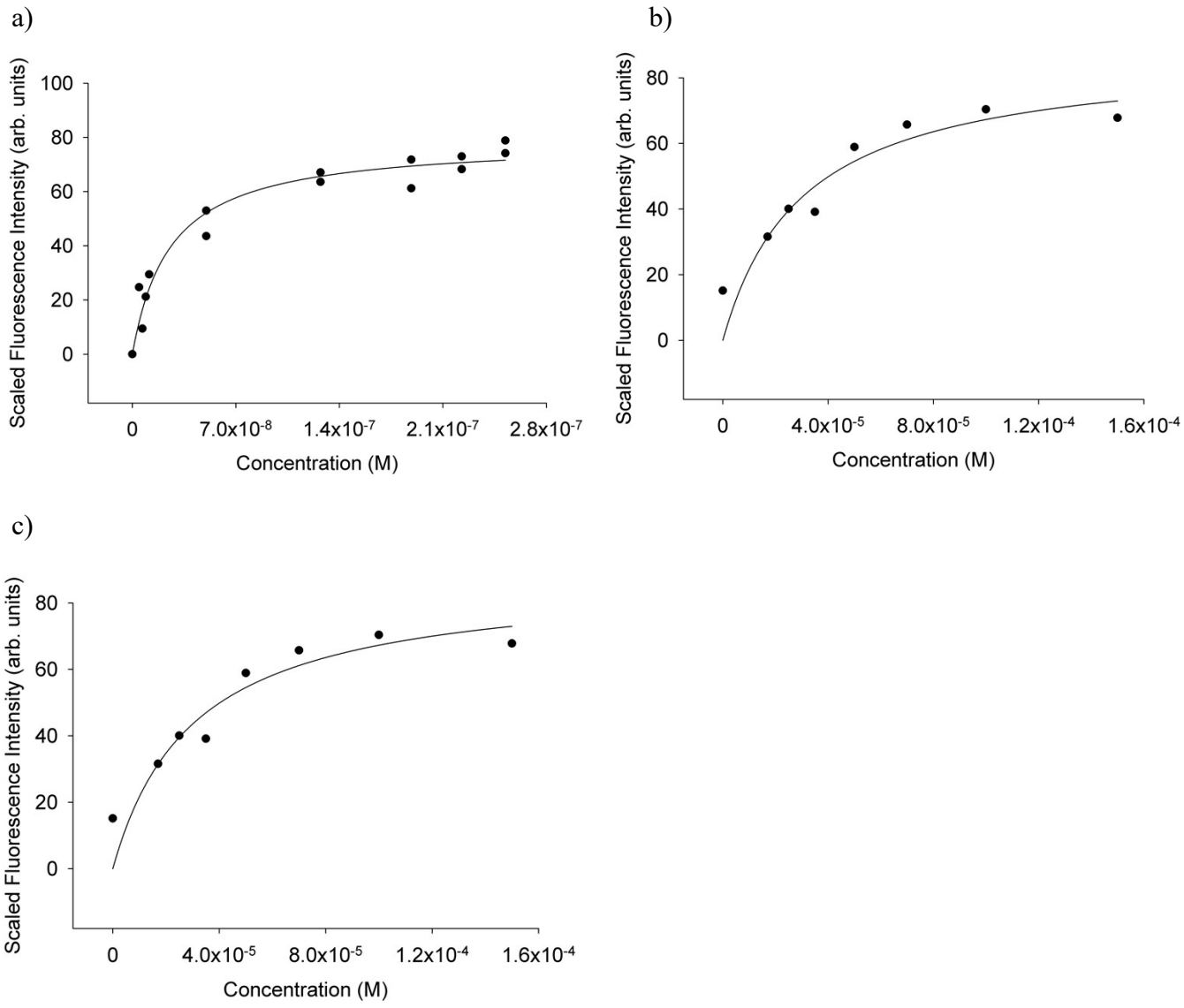

Table S1. Log(K_{OW})'s and experimental solubilities for (A) fluoranthene, (B) pyrene, (C) umbelliferone, (D) phenol red, (E) bisphenol A, (F) naphthalene, (G) anthracene, and (H) IC.

	A	**B**	**C**	**D**	**E**	**F**	**G**	**H**
log(K_{OW})	5.16[2]	4.88[3]	1.58[4]	3.02[5]	3.32[6]	3.30[10]	4.45[7]	-0.22[8]
experimental solubility (μM)	1.29[9]	0.67[3]	N/A	2170[5]	526[18]	249[11]	0.24[7]	N/A

Table S2. Maximum emission wavelengths of fluorescence for fluoranthene, umbelliferone, pyrene, BPA and phenol red when excited at 337 nm,228 nm (for BPA), and 313 nm (for naphthalene). The bolded wavelength for phenol red was that used for the experiments at a singular wavelength.

	Fluoranthene	Umbelliferone	Pyrene	BPA	Phenol Red	**Napthalene**
Emission wavelength	443.3 nm	460 nm	393 nm	341.3 nm	544nm, **545 nm**, 546 nm	350 nm

Table S3. Measured linear ranges of bulk fluorescence of fluoranthene, umbelliferone, pyrene, and naphthalene.

	Fluoranthene	Umbelliferone	Pyrene	BPA	Phenol Red	**Naphthalene**
Linear concentration range in bulk	0 M to 1.29 μM	0 M to ~3 μM	0 M to ~0.02 μM	0 M to ~1.5 mM	0 M to 25 μM	0 M to ~ 0.2 mM

Table S4. The *b* fit parameters for the hyperbolic fits of the combined and normalized freshwater surface datasets.

	b	R^2
fluoranthene	(1.97 +/- 0.70) * 10^{-8}	0.83
pyrene	(2.87 +/- 0.97) * 10^{-9}	0.89
umbelliferone	(1.71 +/- 0.22) * 10^{-6}	0.98
BPA	(7.27 +/- 3.22) * 10^{-6}	0.56
Phenol red	(2.44 +/- 0.44) * 10^{-5}	0.87
anthracene	(2.56 +/- 0.56) *10^{-8}	0.95
IC	(3.05 +/- 1.19) *10^{-5}	0.90
naphthalene	(5.31 +/- 0.58) *10^{-5}	0.98

Table S5. The *b* fit parameters for the hyperbolic fits of the combined and normalized octanol-coated surface datasets.

	b	R^2
fluoranthene	(1.12 +/- 0.23) * 10^{-9}	0.90
pyrene	(1.40 +/- 0.68) * 10^{-11}	0.55
umbelliferone	(3.37 +/- 0.86) * 10^{-6}	0.97
Phenol red	(6.90 +/- 1.02) * 10^{-5}	0.98
IC	(3.08 +/- 0.76) *10^{-5}	0.93
naphthalene	(2.89 +/- 0.72) * 10^{-6}	0.85

SI References

(1) B. Nugroho, Y. Pramudya and W.Widodo, The Content Analysis of Bisphenol A (BPA) on Water in Plastic Glass with Varying Temperatures and Contact Times Using UV-VIS Spectrophotometer. *Indonesian Review of Physics* **2019**, *1* (2), 27. https://doi.org/10.12928/irip.v1i2.263.

(2) Fluoranthene, CSID=8800. *ChemSpider*. Royal Society of Chemistry.

(3) Pyrene, CSID=29153. *ChemSpider*. Royal Society of Chemistry .

(4) Umbelliferone, CSID=4444774. *ChemSpider*. Royal Society of Chemistry.

(5) Phenol Red, CSID=4602. *ChemSpider*. Royal Society of Chemistry.

(6) Bisphenol A, CSID=6371. *ChemSpider*. Royal Society of Chemistry.

(7) Anthracene, CSID=8111. *ChemSpider*. Royal Society of Chemistry.

(8) Imidazole-2-Carbaldehyde, CSID=23329. *ChemSpider*. Royal Society of Chemistry.

(9) D. Mackay,and W.Y. Shiu, Aqueous Solubility of Polynuclear Aromatic Hydrocarbons. *J Chem Eng Data* **1977**, *22* (4), 399–402. https://doi.org/10.1021/je60075a012.

(10) Naphthalene, CSID=906. *ChemSpider.* Royal Society of Chemistry.

(11) R.S. Pearlman, S.H. Yalkowsky and S. Banerjee, Water Solubilities of Polynuclear Aromatic and Heteroaromatic Compounds. *Journal of Physical and Chemical Reference Data*, **1984** *13*(2), 555–562. https://doi.org/10.1063/1.555712