

Supplementary Material for
“An approach for calculating a confidence interval
from a single aquatic sample for
monitoring hydrophobic organic contaminants”

Melissa M. Matzke,^{*†} Sarah E. Allan,[‡] Kim A. Anderson,[‡] and Katrina M. Waters[†]

[†] Computational Biology & Bioinformatics, Pacific Northwest National Laboratory, PO Box 999, Richland, WA, USA

[‡] Department of Environmental and Molecular Toxicology, Oregon State University, Corvallis, OR, USA

^{*} To whom correspondence may be addressed (mmatzke@pnnl.gov)

Table S1. Sampling frequency used in the pilot study of the Portland Harbor Superfund.

	2009		2010		
	Summer Site A	Fall Site A	Summer Site A	Fall Site A	Fall Site B
Number of Sampling Cages	3	5	1	1	1
Number of LFT Samplers Within a Cage	5 ^a	5 ^a	5 ^b	5 ^b	5 ^b

^a Chemically analyzed as a single composite sample.

^b Chemically analyzed as 5 independent samples.

Table S2. Within Sampling Cage Variance. Estimates of variance between LFT within a sampling cage for \log_{10} analyte values. Levene's test is used to test the null hypothesis that the observed within cage variance across the 3 locations are equal.

Chemical	Variance Within Cage			Levene's Test	Pooled Variance Within Cage (Eqn. 1)
	Summer 2010 (r ₁ =5)	Fall 2010 – A (r ₂ =5)	Fall 2010 – B (r ₃ =5)	$H_o : \sigma_1^2 = \sigma_2^2 = \sigma_3^2$ P-Value	
1-Methylphenanthrene	0.0017	0.0014	0.0005	0.137	0.0012
1-Methylpyrene	0.0005	0.0006	0.0046	0.286	0.0019
2-methylanthracene	0.0007	0.0014	0.0016	0.283	0.0012
2-Methylphenanthrene	0.0013	0.0006	0.0020	0.516	0.0013
3,6-Dimethylphenanthrene	Na	Na	0.0001	Na	0.0001
Acenaphthene	0.0054	0.0015	0.0105	0.290	0.0058
Acenaphthylene	0.0017	0.0028	Na	0.583	0.0023
Anthracene	0.0008	0.0006	0.0011	0.787	0.0008
Benz[a]anthracene	0.0003	0.0006	0.0056	0.252	0.0022
Benzo[a]pyrene	0.0001	0.0029	0.0052	0.048	0.0027
Benzo[b]fluoranthene	0.0003	0.0008	0.0095	0.211	0.0035
Benzo[e]pyrene	0.0005	0.0008	0.0051	0.200	0.0021
Benzo[g,h,i]perylene	0.0047	0.0035	0.0005	0.375	0.0029
Benzo[k]fluoranthene	0.0010	0.0007	0.0049	0.306	0.0022
Chrysene	0.0006	0.0002	0.0045	0.223	0.0018
Dibenzothiophene	0.0024	0.0023	0.0057	0.470	0.0035
Fluoranthene	0.0008	0.0004	0.0038	0.281	0.0017
Fluorene	0.0042	0.0014	0.0074	0.411	0.0044
Indeno[1,2,3-c,d]pyrene	0.0002	0.0019	Na	0.060	0.0011
Naphthalene	0.0113	0.0014	0.0021	0.014	0.0052
Naphthalene, 1,6-dimethyl-	0.0028	0.0066	Na	0.211	0.0047
Naphthalene, 1-methyl-	0.0072	0.0015	Na	0.120	0.0044
Naphthalene, 2-methyl-	0.0079	0.0038	0.0053	0.650	0.0057
Phenanthrene	0.0024	0.0008	0.0049	0.341	0.0027
Pyrene	0.0005	0.0009	0.0024	0.422	0.0013
Retene	0.0010	0.0010	0.0012	0.956	0.0011

Table S3. Between Sampling Cage Variance. Estimates of variance between sampling cages. Estimates of the \log_{10} analyte values. Levene's test is used to test the null hypothesis that the observed between cage variance across the 2 locations are equal.

Chemical	Variance Between Cage		Levene's Test	Pooled Variance Between Cage (Eqn. 2)
	Summer 2009 (n ₁ =3 cages)	Fall 2009 (n ₂ =5 cages)	$H_o : \sigma_1^2 = \sigma_2^2$ P-value	
1-Methylphenanthrene	0.0023	0.0018	0.914	0.0020
1-Methylpyrene	0.0076	0.0045	0.670	0.0055
2-methylanthracene	0.0047	0.0017	0.193	0.0027
2-Methylphenanthrene	0.0028	0.0018	0.686	0.0022
3,6-Dimethylphenanthrene	0.0026	0.0018	0.814	0.0020
Acenaphthene	0.0014	0.0034	0.412	0.0027
Acenaphthylene	0.0071	0.0022	0.183	0.0038
Anthracene	0.0050	0.0017	0.205	0.0028
Benz[a]anthracene	0.0058	0.0028	0.357	0.0038
Benzo[a]pyrene	0.0288	0.0121	0.350	0.0176
Benzo[b]fluoranthene	0.0240	0.0054	0.104	0.0116
Benzo[e]pyrene	0.0149	0.0048	0.203	0.0082
Benzo[g,h,i]perylene	0.0634	0.0050	0.049	0.0245
Benzo[k]fluoranthene	0.0268	0.0123	0.433	0.0172
Chrysene	0.0044	0.0030	0.757	0.0035
Dibenzothiophene	0.0029	0.0024	0.993	0.0025
Fluoranthene	0.0033	0.0014	0.315	0.0020
Fluorene	0.0029	0.0028	0.859	0.0029
Indeno[1,2,3-c,d]pyrene	0.0976	0.0048	0.042	0.0357
Naphthalene	0.0029	0.0064	0.122	0.0053
Naphthalene, 1,6-dimethyl-	0.0007	0.0025	0.391	0.0019
Naphthalene, 1-methyl-	0.0010	0.0039	0.430	0.0029
Naphthalene, 2-methyl-	0.0028	0.0050	0.583	0.0043
Phenanthrene	0.0024	0.0017	0.817	0.0019
Pyrene	0.0040	0.0017	0.299	0.0024
Retene	0.0036	0.0020	0.583	0.0025

Table S4. 95% confidence intervals for the log₁₀ mean (pg/μL) based on a single observation sampling events (n=1) at the Portland Harbor Superfund during fall 2009 to fall 2010.

Chemical	Superfund Site 1			Superfund Site 2			Upstream		
	Fall 2009	Summer 2010	Fall 2010	Fall 2009	Summer 2010	Fall 2010	Fall 2009	Summer 2010	Fall 2010
1-Methylphenanthrene	(2.423, 2.598)	(2.553, 2.728)	(2.538, 2.713)	(2.906, 3.082)	(2.788, 2.964)	(3.032, 3.207)	(1.812, 1.988)	Na	(1.801, 1.976)
1-Methylpyrene	(2.143, 2.434)	(1.980, 2.271)	(2.237, 2.528)	(2.701, 2.992)	(2.284, 2.574)	(2.544, 2.834)	(1.377, 1.668)	(1.352, 1.643)	(1.713, 2.003)
2-methylanthracene	(2.141, 2.345)	(2.098, 2.302)	(2.038, 2.241)	(2.614, 2.818)	(2.425, 2.628)	(2.598, 2.802)	(2.114, 2.317)	Na	(1.862, 2.066)
2-Methylphenanthrene	(2.485, 2.668)	(2.568, 2.752)	(2.502, 2.686)	(3.126, 3.31)	(3.017, 3.201)	(3.158, 3.342)	(2.118, 2.302)	(2.188, 2.372)	(2.062, 2.246)
3,6-Dimethylphenanthrene	(2.454, 2.630)	(2.152, 2.327)	Na	(2.719, 2.894)	(2.383, 2.559)	(2.578, 2.753)	Na	(1.795, 1.971)	(2.132, 2.307)
Acenaphthene	(2.416, 2.619)	(2.201, 2.405)	(2.204, 2.408)	(2.747, 2.95)	(2.660, 2.863)	(2.860, 3.064)	Na	(1.637, 1.840)	Na
Acenaphthylene	(1.220, 1.462)	(1.287, 1.529)	(1.562, 1.804)	(1.558, 1.799)	(1.593, 1.835)	(2.059, 2.301)	Na	Na	Na
Anthracene	(2.360, 2.568)	(2.447, 2.654)	(2.328, 2.535)	(2.961, 3.169)	(2.829, 3.037)	(2.938, 3.145)	(1.454, 1.661)	(1.767, 1.974)	(1.731, 1.938)
Benz[<i>a</i>]anthracene	(2.754, 2.996)	(2.657, 2.899)	(2.790, 3.031)	(3.337, 3.579)	(2.904, 3.146)	(3.315, 3.556)	(2.358, 2.599)	(1.856, 2.097)	(2.280, 2.522)
Benzo[<i>a</i>]pyrene	(1.807, 2.327)	(1.450, 1.970)	Na	(2.367, 2.887)	(1.861, 2.381)	(2.422, 2.942)	Na	(0.697, 1.217)	Na
Benzo[<i>b</i>]fluoranthene	(1.981, 2.403)	(1.728, 2.150)	(2.227, 2.649)	(2.596, 3.018)	(2.094, 2.516)	(2.668, 3.09)	(1.183, 1.605)	(0.917, 1.339)	(1.717, 2.139)
Benzo[<i>e</i>]pyrene	(1.991, 2.346)	(1.829, 2.184)	Na	(2.466, 2.821)	(2.104, 2.459)	(2.326, 2.681)	(1.675, 2.03)	(1.301, 1.656)	Na
Benzo[<i>g,h,i</i>]perylene	(1.293, 1.906)	(1.064, 1.678)	(1.427, 2.04)	(1.803, 2.417)	(1.373, 1.986)	(1.863, 2.477)	(0.825, 1.439)	(0.636, 1.25)	(1.302, 1.916)
Benzo[<i>k</i>]fluoranthene	(1.926, 2.44)	(1.053, 1.567)	(1.754, 2.268)	(2.056, 2.57)	(1.556, 2.070)	(2.214, 2.728)	(0.689, 1.204)	Na	(1.281, 1.795)
Chrysene	(2.919, 3.151)	(2.743, 2.975)	(3.043, 3.275)	(3.402, 3.633)	(3.032, 3.264)	(3.430, 3.662)	(2.042, 2.274)	(2.020, 2.252)	(2.542, 2.774)
Dibenzothiophene	(2.049, 2.245)	(1.939, 2.135)	(2.000, 2.196)	(2.695, 2.891)	(2.478, 2.674)	(2.695, 2.891)	Na	(1.281, 1.477)	Na
Fluoranthene	(3.749, 3.924)	(3.508, 3.683)	(3.682, 3.858)	(4.144, 4.319)	(3.810, 3.985)	(4.160, 4.335)	(2.638, 2.813)	(2.693, 2.868)	(2.936, 3.112)
Fluorene	(2.509, 2.72)	(2.188, 2.399)	(2.281, 2.492)	(2.670, 2.882)	(2.536, 2.747)	(2.848, 3.060)	(1.468, 1.679)	(1.823, 2.034)	(1.724, 1.935)
Indeno[<i>1,2,3-c,d</i>]pyrene	(0.989, 1.729)	(0.870, 1.611)	(1.084, 1.825)	(1.437, 2.178)	(1.063, 1.803)	(1.536, 2.277)	Na	Na	(0.831, 1.571)
Naphthalene	(1.419, 1.704)	(1.526, 1.811)	(1.906, 2.192)	(1.673, 1.958)	(1.962, 2.247)	(2.900, 3.186)	(0.986, 1.271)	(1.499, 1.784)	(1.753, 2.038)
Naphthalene, 1,6-dimethyl-	(1.650, 1.821)	(1.646, 1.817)	(1.777, 1.948)	(2.073, 2.244)	(2.243, 2.414)	(2.266, 2.436)	(1.430, 1.601)	(1.932, 2.103)	(1.655, 1.826)
Naphthalene, 1-methyl-	(1.711, 1.922)	(1.829, 2.04)	(1.771, 1.982)	(1.890, 2.101)	(2.162, 2.373)	(2.575, 2.786)	(1.381, 1.592)	(1.915, 2.126)	(1.762, 1.973)
Naphthalene, 2-methyl-	(1.789, 2.046)	(1.918, 2.175)	(1.858, 2.115)	(1.914, 2.171)	(2.274, 2.531)	(2.770, 3.027)	(1.535, 1.792)	(2.010, 2.267)	(1.968, 2.225)
Phenanthrene	(3.037, 3.208)	(3.048, 3.219)	(2.875, 3.046)	(3.660, 3.831)	(3.524, 3.695)	(3.598, 3.769)	(2.045, 2.216)	(2.534, 2.705)	(1.958, 2.128)
Pyrene	(3.780, 3.972)	(3.539, 3.731)	(3.704, 3.896)	(4.194, 4.386)	(3.834, 4.026)	(4.169, 4.361)	(2.620, 2.812)	(2.660, 2.852)	(3.056, 3.248)
Retene	(3.085, 3.281)	(2.940, 3.136)	(3.111, 3.307)	(3.122, 3.318)	(2.980, 3.176)	(3.242, 3.438)	(2.518, 2.714)	(2.626, 2.822)	(3.074, 3.27)