

SUPPLEMENTARY INFORMATION

Table S1) Method Performance for TPAH in Surface Water

Table S1a) The Method Detection Limit (MDL) for low level surface water was determined by spiking 50 mL of DI water with 0.05 mL of 20 µg/L PAH mixture to provide a nominal PAH concentration of 0.02 µg/L (0.02 ppb) level for each component. Replicate analysis (N=8) provided the following data.

Compound	Detected Total Concentration (µg/L)								Average % Recovery	Mean (µg/L)	Std. Dev.	% Rel. Std. Dev.	Expanded Measurement Uncertainty (EMU)
	S1	S2	S3	S4	S5	S6	S7	S8					
Acenaphthene	0.019	0.020	0.020	0.020	0.019	0.019	0.019	0.021	98	0.020	8.03e-4	4.1	0.080
Acenaphthylene	0.019	0.021	0.021	0.020	0.020	0.020	0.019	0.019	100	0.020	8.57e-4	4.3	0.084
Anthracene	0.020	0.020	0.021	0.020	0.021	0.021	0.020	0.021	102	0.020	5.22e-4	2.6	0.069
Benzo(a)anthracene	0.018	0.018	0.019	0.018	0.018	0.018	0.019	0.019	91	0.018	4.47e-4	2.4	0.105
Benzo(a)pyrene	0.018	0.019	0.020	0.019	0.018	0.018	0.021	0.020	95	0.019	9.09e-4	4.8	0.162
Benzo(e)pyrene	0.019	0.021	0.020	0.018	0.019	0.019	0.019	0.021	98	0.020	8.25e-4	4.2	0.171
Benzo(b)fluoranthene	0.021	0.022	0.020	0.020	0.020	0.020	0.018	0.021	101	0.020	9.81e-4	4.9	0.018
Benzo(g,h,i)perylene	0.020	0.020	0.020	0.019	0.019	0.020	0.021	0.021	101	0.020	7.55e-4	3.7	0.054
Benzo(k)fluoranthene	0.020	0.021	0.020	0.020	0.020	0.019	0.021	0.021	101	0.020	4.36e-4	2.2	0.097
Chrysene	0.019	0.020	0.020	0.020	0.020	0.020	0.020	0.021	100	0.020	4.42e-4	2.2	0.171
Dibenzo(a,h)anthracene	0.020	0.020	0.020	0.020	0.020	0.020	0.020	0.020	100	0.020	2.47e-4	1.2	0.148
Fluoranthene	0.019	0.019	0.020	0.020	0.020	0.020	0.020	0.020	99	0.020	3.79e-4	1.9	0.049
Fluorene	0.021	0.019	0.021	0.021	0.019	0.021	0.020	0.020	101	0.020	7.88e-4	3.9	0.252
Indeno(1,2,3-cd)pyrene	0.019	0.019	0.020	0.019	0.020	0.019	0.019	0.018	96	0.019	6.71e-4	3.5	0.175
Naphthalene	0.019	0.019	0.019	0.020	0.019	0.019	0.021	0.019	97	0.019	6.17e-4	3.2	0.032
Perylene	0.017	0.018	0.018	0.018	0.018	0.017	0.019	0.017	89	0.018	7.54e-4	4.2	0.090
Phenanthrene	0.020	0.018	0.019	0.019	0.018	0.018	0.019	0.019	94	0.019	6.04e-4	3.2	0.087
Pyrene	0.020	0.019	0.019	0.020	0.019	0.019	0.020	0.020	97	0.019	3.33e-4	1.7	0.029

Table S1b) Middle Level Determination for Surface Water Samples. Replicate analysis (N=8) of blank DI water spiked at 0.2 µg/L (0.2 ppb) with a laboratory prepared standard.

Compound	Detected Total Concentration (µg/L)								Average % Recovery	Mean (µg/L)	Std. Dev.	% Rel. Std. Dev.	Expanded Measurement Uncertainty (EMU)
	S1	S2	S3	S4	S5	S6	S7	S8					
Acenaphthene	0.199	0.191	0.184	0.184	0.189	0.199	0.191	0.179	98	0.189	7.13e-3	3.8	0.080
Acenaphthylene	0.206	0.208	0.207	0.189	0.206	0.203	0.188	0.198	93	0.201	8.21e-3	4.1	0.084
Anthracene	0.198	0.190	0.190	0.184	0.186	0.189	0.189	0.195	92	0.190	4.63e-3	2.4	0.069
Benzo(a)anthracene	0.194	0.175	0.185	0.185	0.189	0.182	0.181	0.195	98	0.186	6.47e-3	3.5	0.105
Benzo(a)pyrene	0.195	0.185	0.180	0.177	0.186	0.185	0.179	0.193	95	0.185	6.38e-3	3.4	0.162
Benzo(e)pyrene	0.198	0.191	0.185	0.188	0.196	0.194	0.193	0.203	108	0.194	5.76e-3	3.0	0.171
Benzo(b)fluoranthene	0.203	0.195	0.188	0.192	0.197	0.197	0.190	0.202	114	0.195	5.29e-3	2.7	0.018
Benzo(g,h,i)perylene	0.196	0.189	0.186	0.185	0.191	0.189	0.184	0.195	98	0.189	4.59e-3	2.4	0.054
Benzo(k)fluoranthene	0.202	0.191	0.192	0.191	0.196	0.196	0.192	0.202	100	0.195	4.35e-3	2.2	0.097
Chrysene	0.197	0.181	0.183	0.185	0.188	0.184	0.186	0.191	97	0.187	5.20e-3	2.8	0.171
Dibenzo(a,h)anthracene	0.196	0.184	0.187	0.180	0.187	0.184	0.183	0.188	83	0.186	4.81e-3	2.6	0.148
Fluoranthene	0.201	0.192	0.194	0.194	0.199	0.193	0.191	0.205	104	0.196	4.97e-3	2.5	0.049
Fluorene	0.198	0.201	0.206	0.201	0.199	0.201	0.197	0.189	94	0.199	4.69e-3	2.4	0.252
Indeno(1,2,3-cd)pyrene	0.166	0.174	0.187	0.187	0.185	0.172	0.168	0.179	85	0.177	8.31e-3	4.7	0.175
Naphthalene	0.206	0.188	0.185	0.182	0.193	0.193	0.191	0.178	85	0.189	8.58e-3	4.5	0.032
Perylene	0.204	0.187	0.184	0.190	0.190	0.192	0.189	0.200	96	0.192	6.62e-3	3.5	0.090
Phenanthrene	0.188	0.189	0.190	0.187	0.188	0.187	0.178	0.181	80	0.186	4.07e-3	2.2	0.087
Pyrene	0.200	0.190	0.194	0.193	0.197	0.192	0.190	0.201	101	0.195	4.10e-3	2.1	0.029

Table S1c) High level Determination for Surface water Samples. Replicate analysis (N=8) of blank DI water spiked at 40 µg/L (40 ppb) with a laboratory prepared standard.

Compound	Detected Total Concentration (µg/L)								Average % Recovery	Mean (µg/L)	Std. Dev.	% Rel. Std. Dev.	Expanded Measurement Uncertainty (EMU)
	S1	S2	S3	S4	S5	S6	S7	S8					
Acenaphthene	39.7	40.5	40.0	38.6	38.7	40.2	40.1	40.0	99	39.7	0.705	1.8	1.437
Acenaphthylene	41.3	42.2	42.2	40.3	40.8	42.2	42.3	42.3	104	41.7	0.788	1.9	1.609

Anthracene	37.8	38.4	38.4	39.7	39.1	39.7	39.6	39.7	98	39.1	0.749	1.9	0.822
Benzo(a)anthracene	39.1	39.4	39.5	40.4	40.3	40.7	40.5	40.3	100	40.0	0.574	1.4	4.632
Benzo(a)pyrene	39.3	39.7	40.0	40.8	40.7	40.9	40.4	40.8	101	40.3	0.603	1.5	1.597
Benzo(e)pyrene	39.4	39.7	40.1	40.8	40.5	40.9	40.6	40.3	101	40.3	0.529	1.3	1.924
Benzo(b)fluoranthene	38.9	39.2	39.4	40.0	39.9	40.1	39.9	40.0	99	39.7	0.447	1.1	2.049
Benzo(g,h,i)perylene	38.6	39.0	39.5	39.8	40.0	39.7	39.6	39.7	99	39.5	0.469	1.2	2.925
Benzo(k)fluoranthene	38.1	38.5	38.9	39.6	39.4	39.5	39.3	39.6	98	39.1	0.539	1.4	1.122
Chrysene	38.5	39.0	39.0	39.9	39.8	40.0	40.0	39.8	99	39.5	0.577	1.5	1.594
Dibenzo(a,h)anthracene	37.8	38.1	38.6	39.0	39.3	39.2	38.8	39.0	97	38.7	0.537	1.4	4.695
Fluoranthene	38.5	38.8	39.3	39.4	39.8	39.8	39.8	39.6	98	39.4	0.505	1.3	0.714
Fluorene	40.7	41.5	40.5	41.1	41.3	41.4	41.0	41.0	103	41.1	0.334	0.8	1.816
Indeno(1,2,3-cd)pyrene	37.7	37.9	38.4	38.9	39.3	38.9	38.8	38.9	96	38.6	0.555	1.4	6.109
Naphthalene	40.2	40.2	40.7	38.1	38.2	41.1	40.9	41.1	100	40.1	1.233	3.1	0.368
Perylene	38.8	39.3	39.5	40.6	40.7	40.8	40.4	40.6	100	40.1	0.753	1.9	4.300
Phenanthrene	38.3	39.0	38.9	39.5	39.6	39.7	39.7	39.9	98	39.3	0.540	1.4	0.917
Pyrene	38.4	38.7	39.0	39.2	39.8	39.8	39.7	39.4	98	39.2	0.527	1.3	0.456

Table S2) PAH Concentrations (ng/mL) and % Recovery of 16 PAHs of 2 QA Water Samples (V16F039_01, V16F039_03) Supplied by CALA (2016) Comparing 1 Step ACN/DCM, 1 Step DCM Only and 2 Step DCM Only Extractions.

Compound	PAH Concentrations in Sample (µg/L)						Average % Recovery for 1 Step ACN/DCM	Average % Recovery for 1 Step DCM	Average % Recovery for 2 Step DCM
	1 Step ACN/DCM		1 Step DCM		2 Step DCM				
	V16F039_01	V16F039_03	V16F039_01	V16F039_03	V16F039_01	V16F039_03			
Acenaphthene	2.20	6.31	1.82	4.94	2.28	7.13	106	86	115
Acenaphthylene	0.88	5.55	0.83	4.07	0.93	6.02	117	99	125
Anthracene	1.32	4.62	1.15	3.40	1.40	5.22	104	84	113
Benzo(a)anthracene	3.63	6.46	3.01	4.28	3.43	6.72	107	81	106
Benzo(a)pyrene	3.65	9.43	2.68	4.85	3.04	7.55	122	77	99
Benzo(b)fluoranthene	3.26	8.29	2.39	5.03	2.76	7.18	125	84	107
Benzo(g,h,i)perylene	1.97	7.55	1.88	5.00	1.80	6.63	108	88	96
Benzo(k)fluoranthene	1.64	9.70	1.37	6.64	1.49	8.99	99	75	91
Chrysene	2.25	8.79	1.78	6.17	1.67	8.63	110	83	94
Dibenzo(a,h)anthracene	3.33	9.04	2.93	5.50	2.86	7.73	109	81	93
Fluoranthene	0.56	5.54	0.66	4.60	0.58	5.88	96	97	101
Fluorene	2.60	4.81	2.08	3.82	2.57	5.53	104	83	111
Indeno(1,2,3-cd)pyrene	2.34	7.35	1.97	4.16	2.30	6.02	109	77	98
Naphthalene	0.84	6.81	0.69	5.24	0.85	7.89	120	95	130
Phenanthrene	1.94	4.92	1.66	3.91	2.02	4.99	104	86	107
Pyrene	1.88	5.09	1.76	4.29	2.02	5.53	94	83	101

Table S3) CALA January 2017 Proficiency testing results of 4 samples (C07-1, C07-2, C07-3, C07-4) with a score of 84-96.

Compound	Assigned Concentration (µg/L)				Reported Concentration (µg/L)				Score
	C07-1	C07-2	C07-3	C07-4	C07-1	C07-2	C07-3	C07-4	
Acenaphthene	0.947	2.88	5.88	7.56	1.103	3.305	6.589	8.693	87
Acenaphthylene	2.43	3.96	5.37	7.73	2.802	4.467	5.611	8.454	92
Anthracene	3.16	4.67	5.26	7.67	4.117	5.482	5.810	9.104	87
Benzo(a)anthracene	1.34	3.32	9.26	9.81	1.380	2.883	9.804	10.475	96
Benzo(a)pyrene	1.28	3.73	10.40	13.00	1.207	2.950	10.875	14.261	96
Benzo(b)fluoranthene	1.95	4.34	7.96	11.00	2.016	3.613	8.677	12.023	95
Benzo(g,h,i)perylene	0.887	4.81	8.73	13.20	0.783	4.443	11.433	16.698	92
Benzo(k)fluoranthene	3.38	4.75	8.99	10.90	3.099	4.166	11.451	14.665	91
Chrysene	1.13	4.01	7.57	9.53	1.080	3.153	8.057	11.444	84
Dibenzo(a,h)anthracene	3.82	5.81	9.98	13.7	3.734	5.301	12.478	16.520	94
Fluoranthene	1.77	2.28	5.51	9.30	1.954	2.346	5.534	9.851	96
Fluorene	0.918	3.39	7.19	8.87	1.040	3.757	7.827	9.885	91
Indeno(1,2,3-cd)pyrene	1.52	3.78	6.70	11.00	1.313	2.848	7.371	12.085	93
Naphthalene	1.16	2.70	5.52	5.66	1.385	3.216	6.403	6.661	89
Phenanthrene	2.30	2.31	5.35	6.85	2.758	2.712	6.171	7.913	86
Pyrene	0.988	3.37	5.92	6.79	1.111	3.582	6.141	7.207	94

Table S4) 18 PAH Concentrations ($\mu\text{g/L}$) in CEWAF prepared at 0.025 g/L, 0.05 g/L and 0.1 g/L of Corexit oil dispersant and 0.25 g/L, 0.5 g/L and 1 g/L of oil at T=0 respectively.

Compound	PAH Concentration ($\mu\text{g/L}$)		
	0.025 g/L Corexit 0.25 g/L oil, T=0hr.	0.05 g/L Corexit 0.5 g/L oil, T=0hr.	0.1 g/L Corexit 1 g/L oil, T=0hr.
Acenaphthene	0.030	0.194	4.283
Acenaphthylene	0.025	0.054	0.000
Anthracene	0.002	0.017	1.205
Benzo(a)anthracene	0.010	0.016	1.762
Benzo(a)pyrene	0.002	0.004	0.524
Benzo(b)fluoranthene	0.014	0.014	1.243
Benzo(g,h,i)perylene	0.025	0.020	3.278
Benzo(k)fluoranthene	0.007	0.007	0.930
Chrysene	0.014	0.018	0.103
Dibenzo(a,h)anthracene	0.079	0.145	10.159
Fluoranthene	0.010	0.011	0.451
Fluorene	0.021	0.020	0.829
Indeno(1,2,3-cd)pyrene	0.305	0.426	23.920
Naphthalene	0.009	0.012	0.397
Phenanthrene	12.019	18.379	269.571
Pyrene	0.014	0.013	0.366

Table S5) Comparison of S/N and area of a CEWAF water sample (0.25 g/L oil and 0.025 g/L dispersant, T=96 hrs) run on both GC/MS SIM and GC/MS/MS PMRM instrumentation. Improvements of S/N and sensitivity using GC/MS/MS PMRM are shown. ND = not detected.

Compound	S/N		Area Count	
	GC/MS [SIM]	GC/MS/MS [PMRM]	GC/MS [SIM]	GC/MS/MS [PMRM]
Naphthalene	6	10.8	649	4654
Acenaphthylene	ND	4.4	ND	1250
Acenaphthene	ND	ND	ND	ND
Fluorene	ND	ND	ND	ND
Phenanthrene	6	6.6	1569	6543
Anthracene	ND	ND	ND	ND
Fluoranthene	ND	ND	ND	ND
Pyrene	4	11.9	2388	13529
Benzo(a)anthracene	4	4.1	1151	8792
Chrysene	27.3	33.6	7995	52236
Benzo(b)fluoranthene	1.3	3.5	1304	8954
Benzo(k)fluoranthene	ND	ND	ND	ND
Benzo(e)pyrene	3.2	10.7	3096	28111
Benzo(a)pyrene	ND	ND	ND	ND
Perylene	ND	ND	ND	ND
Indeno(1,2,3-cd)pyrene	ND	ND	ND	ND
Dibenzo(a,h)anthracene	3.7	3.9	603	4917
Benzo(g,h,i)perylene	8.5	15.8	1447	9974

Figure S1) Collision Gas comparison: Response area counts at high PAH concentrations of 2000 µg/L in DCM using Helium vs Nitrogen as Collision

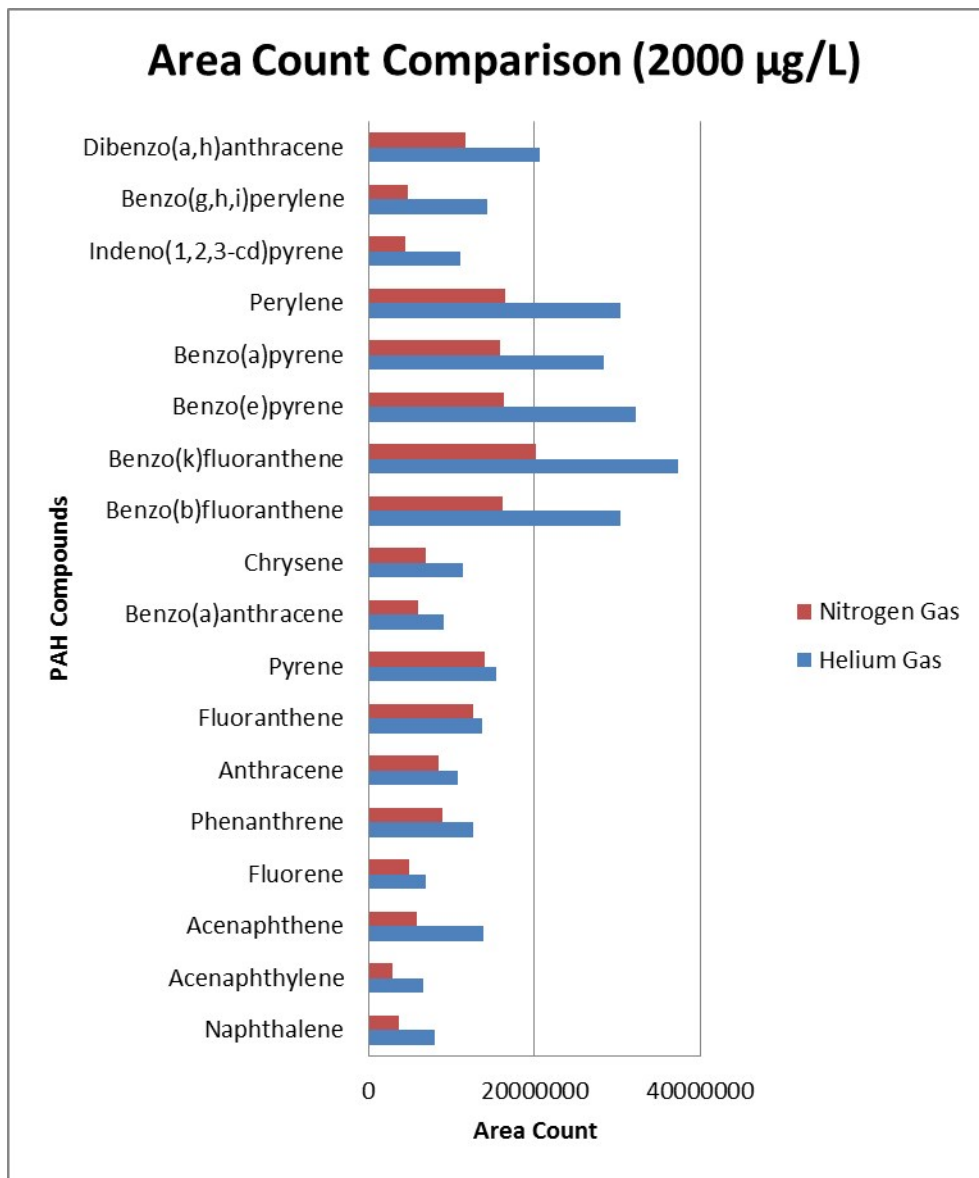


Figure S2): Extracted Ion Chromatogram of ion 128 m/z showing interference peaks derived from sample extraction in plastic tubes. Integration and recovery of naphthalene is severely affected due to interferences compared to the clean baseline of glass.

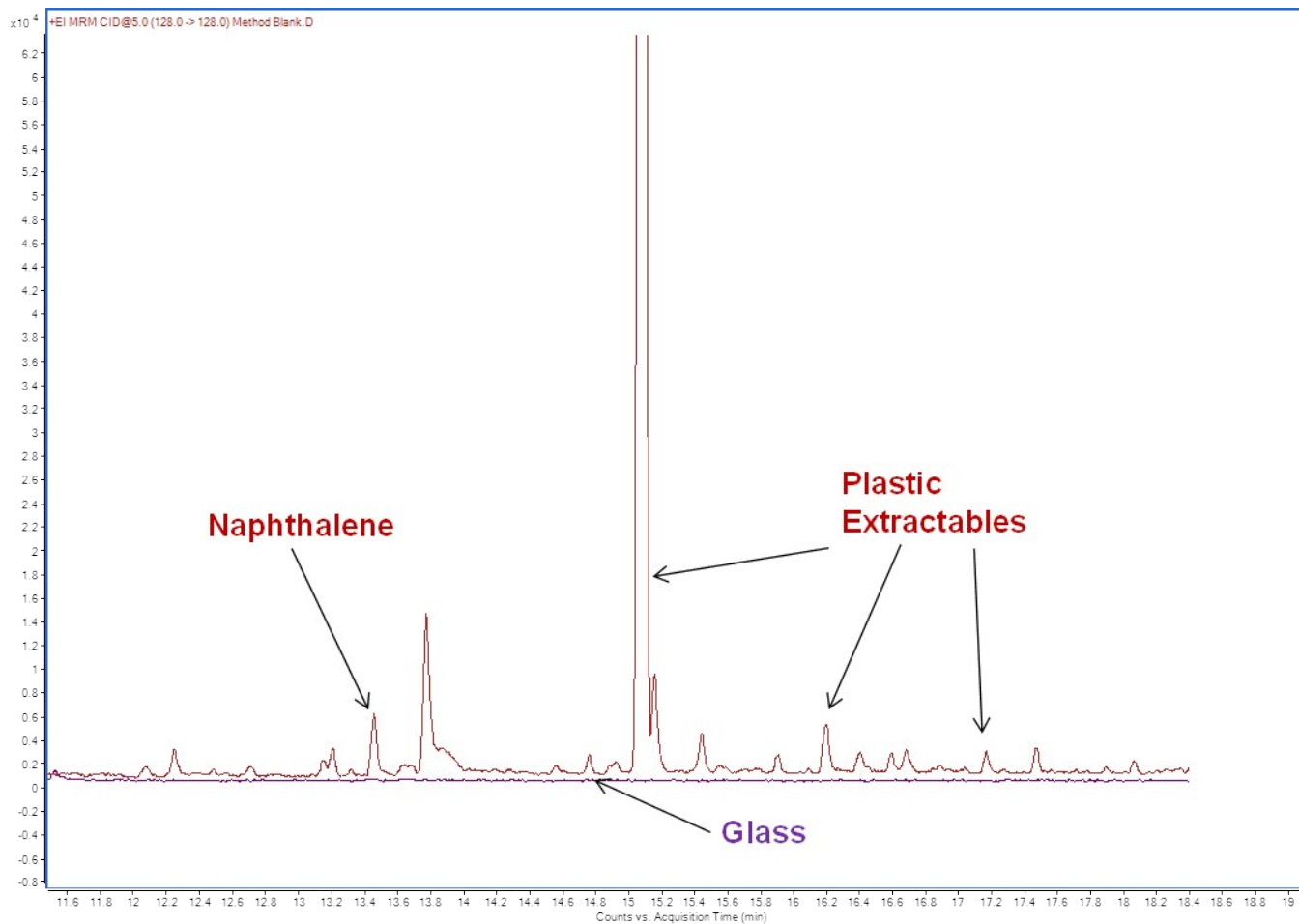
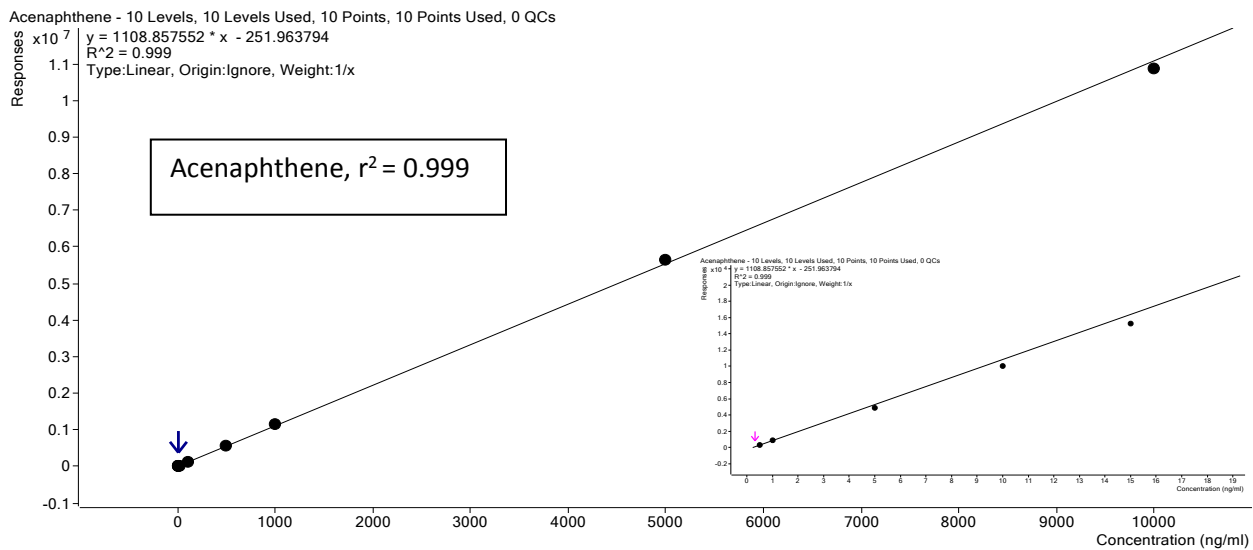
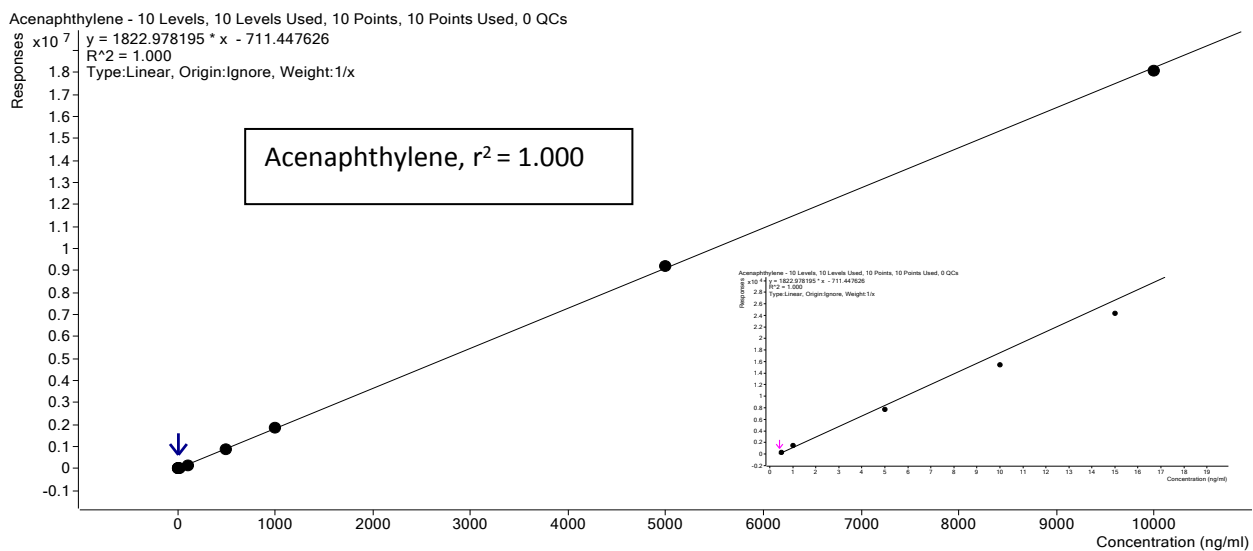
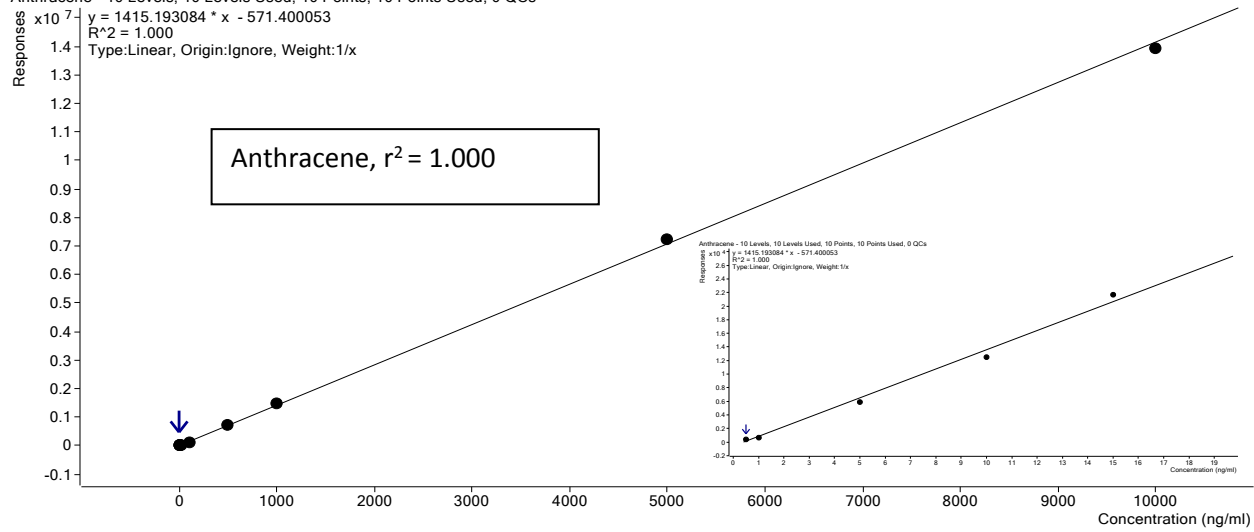


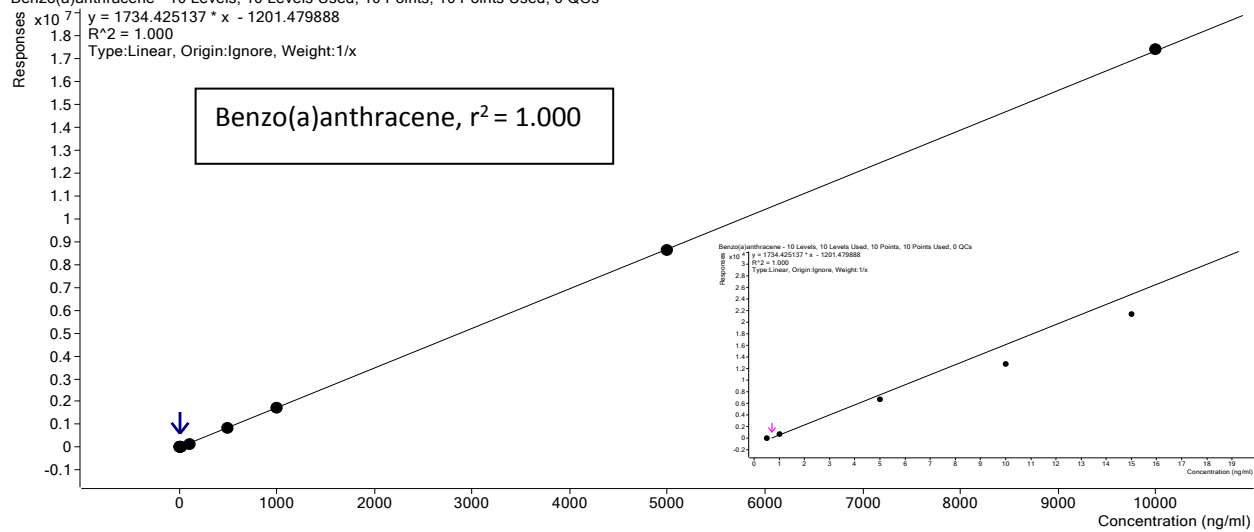
Figure S3) 18 PAH linear calibration curves from 0.5 µg/L to 10000 µg/L showing linearity with r^2 values of > 0.995. 5 of the bottom end calibration points are also shown to scale to demonstrate linearity of both low and high concentrations.



Anthracene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs
 $y = 1415.193084 * x - 571.400053$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x

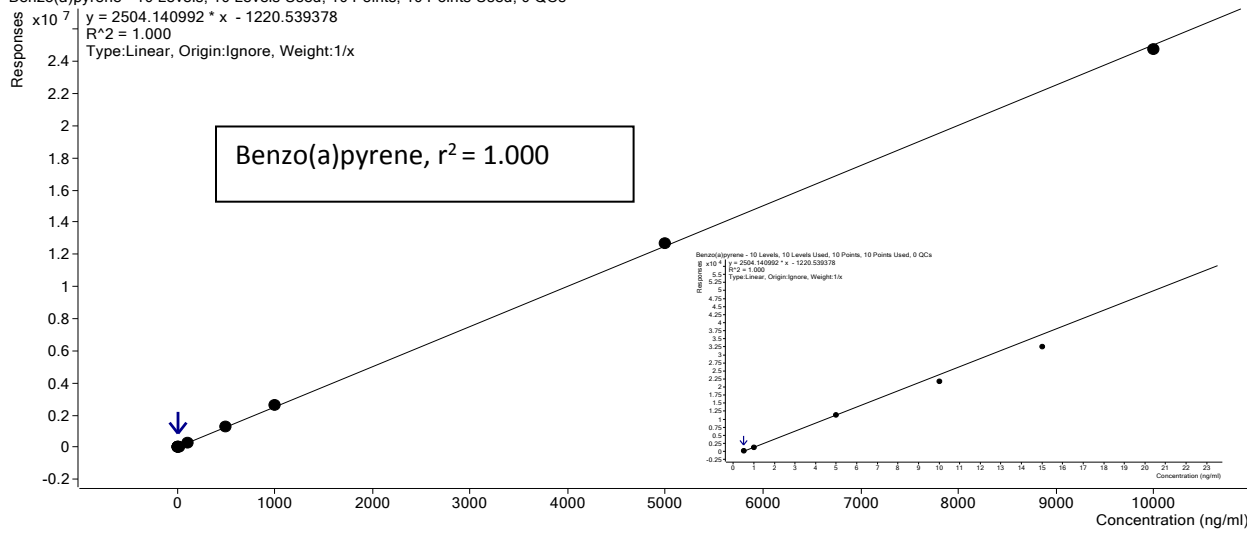


Benzo(a)anthracene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs
 $y = 1734.425137 * x - 1201.479888$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x



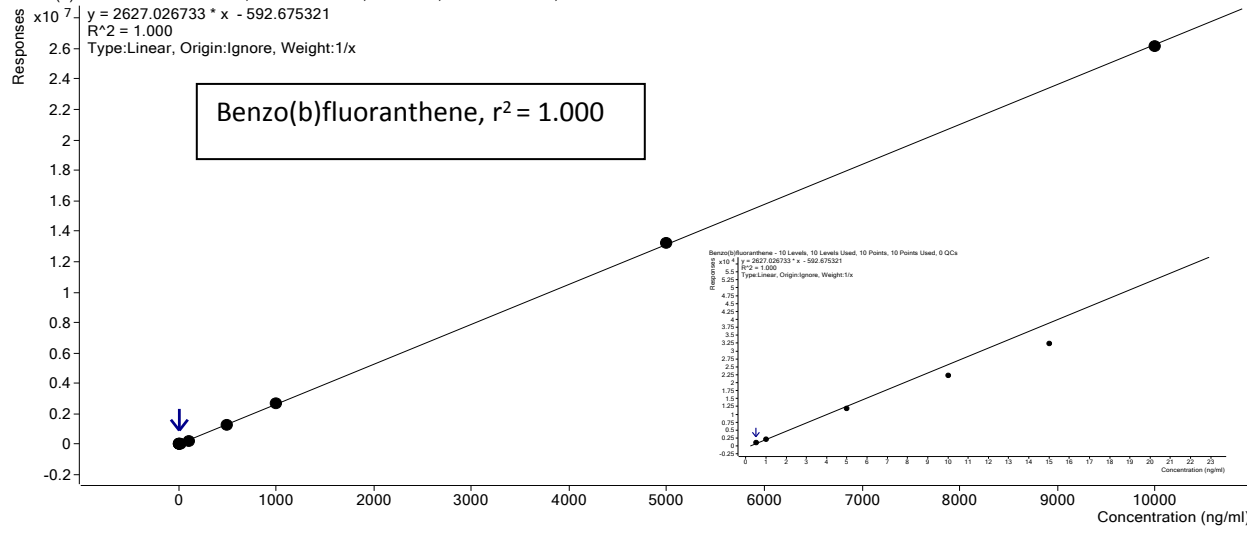
Benzo(a)pyrene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 2504.140992 \cdot x - 1220.539378$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x



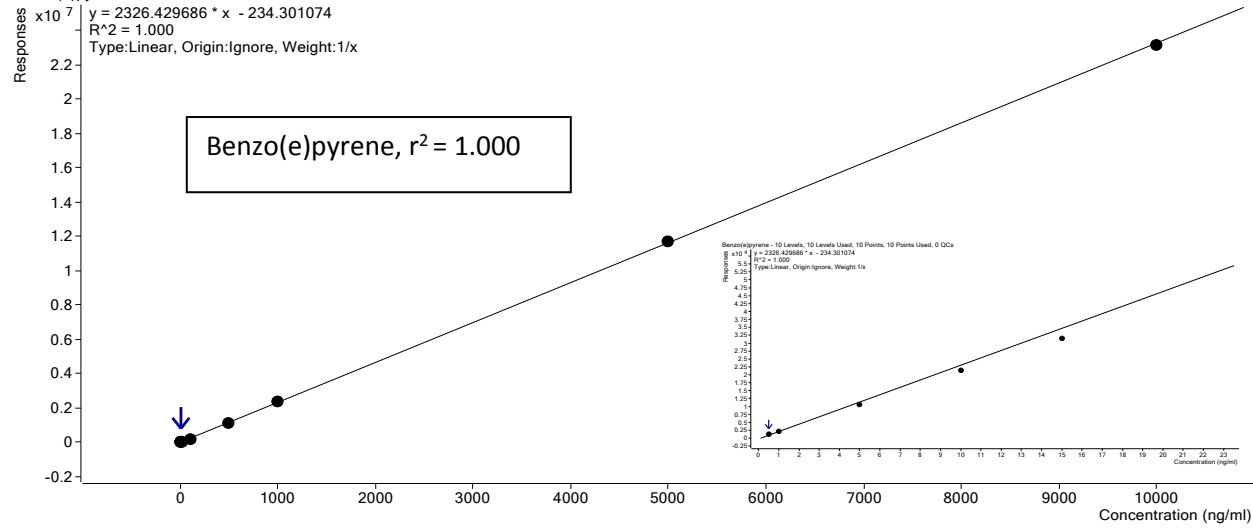
Benzo(b)fluoranthene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 2627.026733 \cdot x - 592.675321$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x



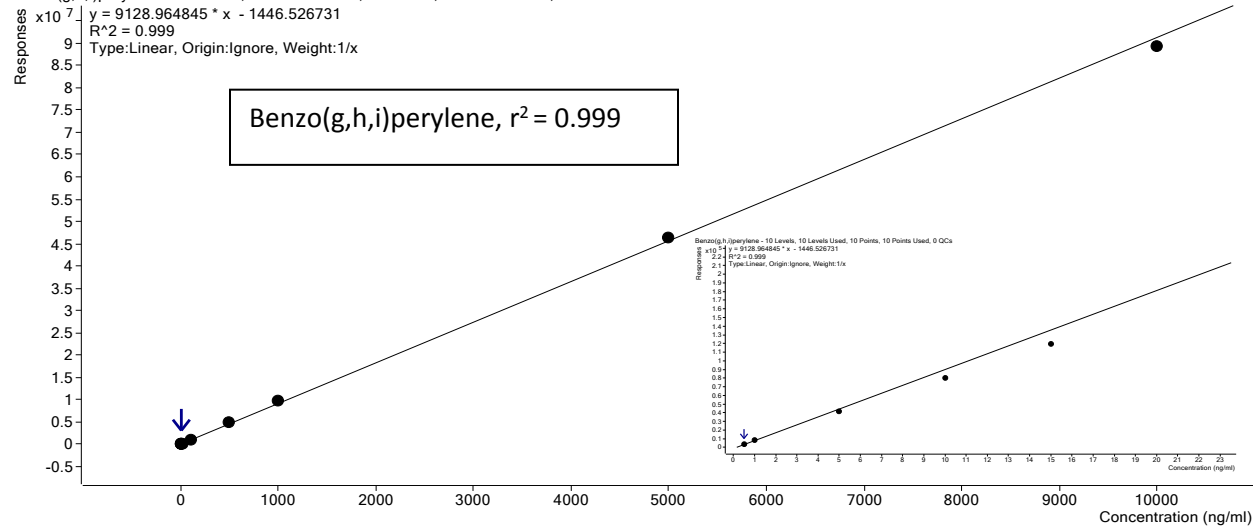
Benzo(e)pyrene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 2326.429686 \cdot x - 234.301074$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x



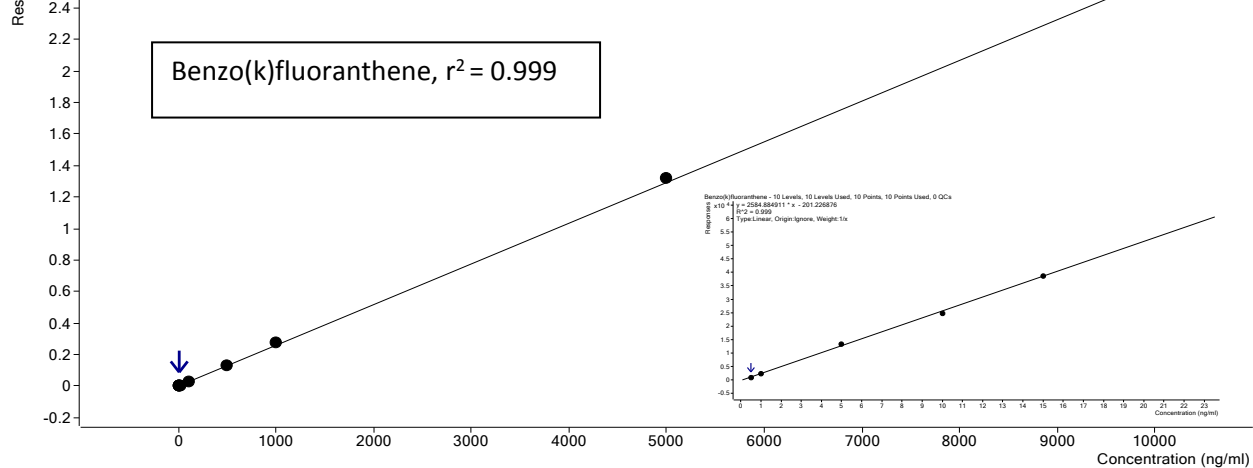
Benzo(g,h,i)perylene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 9128.964845 \cdot x - 1446.526731$
 $R^2 = 0.999$
Type:Linear, Origin:Ignore, Weight:1/x



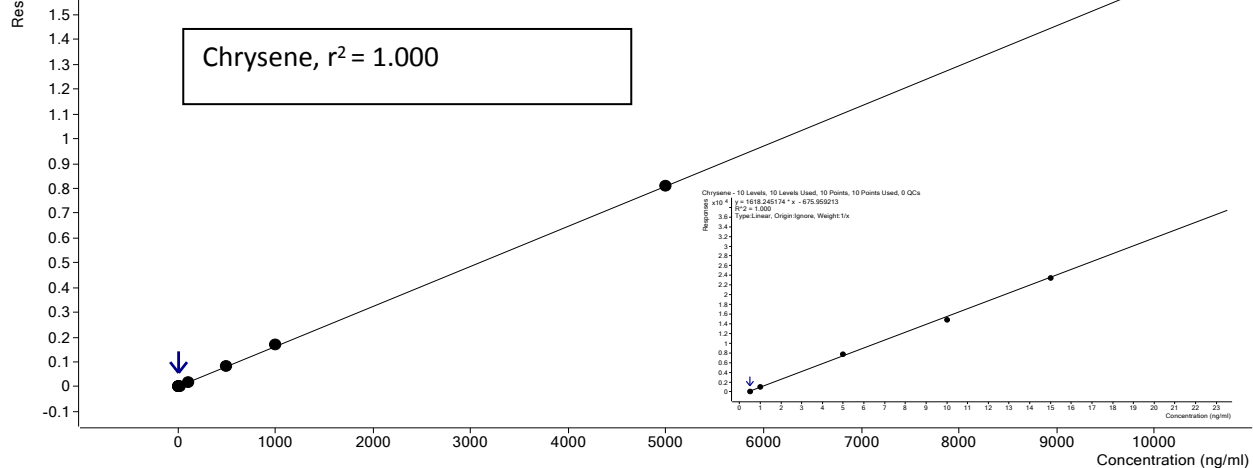
Benzo(k)fluoranthene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 2584.884911 * x - 201.226876$
 $R^2 = 0.999$
Type:Linear, Origin:Ignore, Weight:1/x



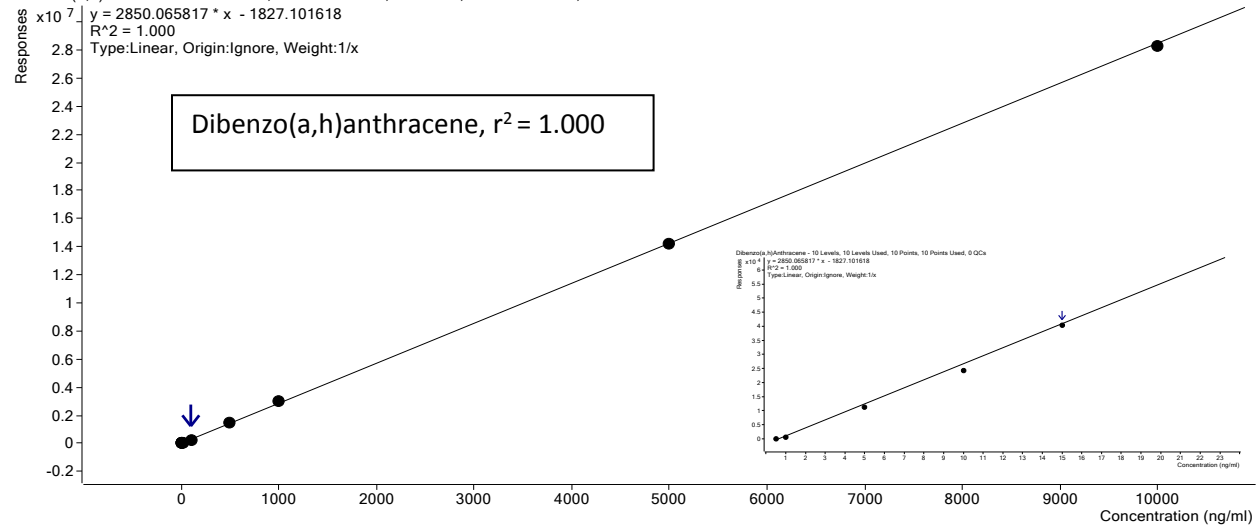
Chrysene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 1618.245174 * x - 675.959213$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x



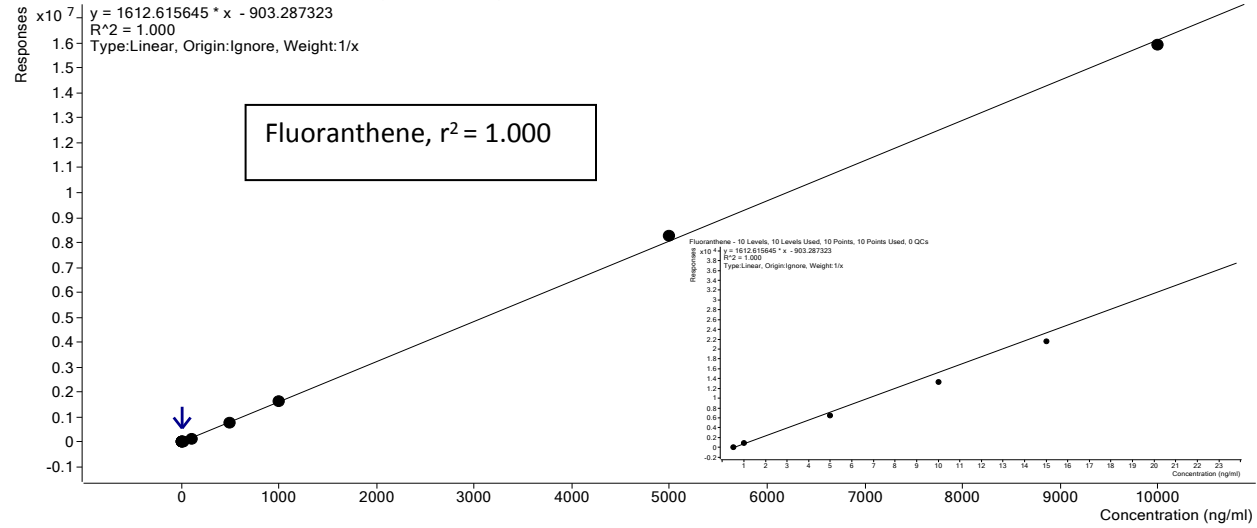
Dibenzo(a,h)Anthracene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 2850.065817 * x - 1827.101618$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x



Fluoranthene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 1612.615645 * x - 903.287323$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x

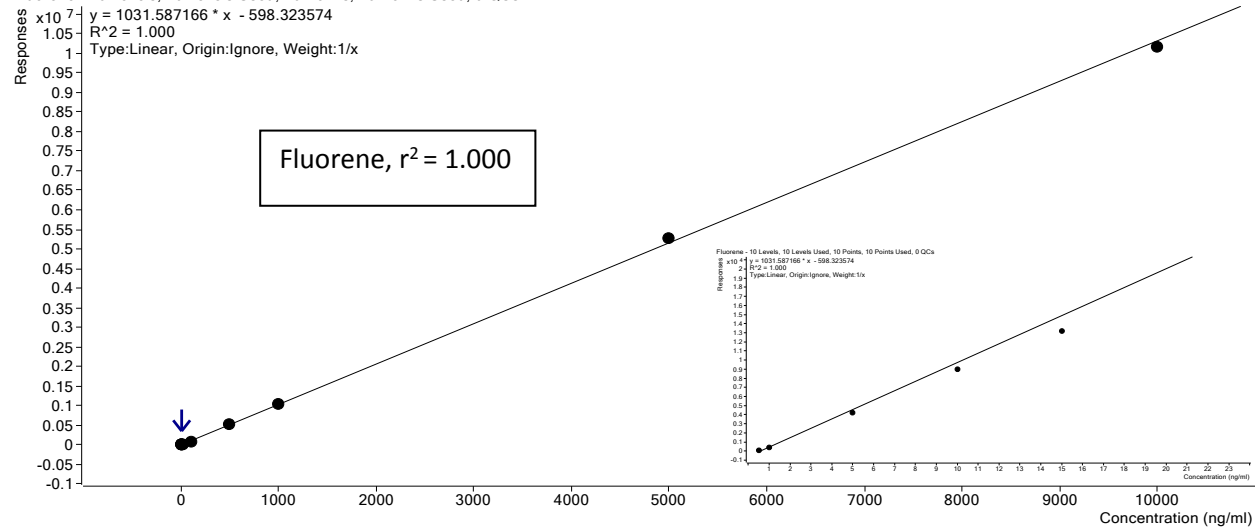


Fluorene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$$y = 1031.587166 \cdot x - 598.323574$$

$R^2 = 1.000$

Type:Linear, Origin:Ignore, Weight:1/x

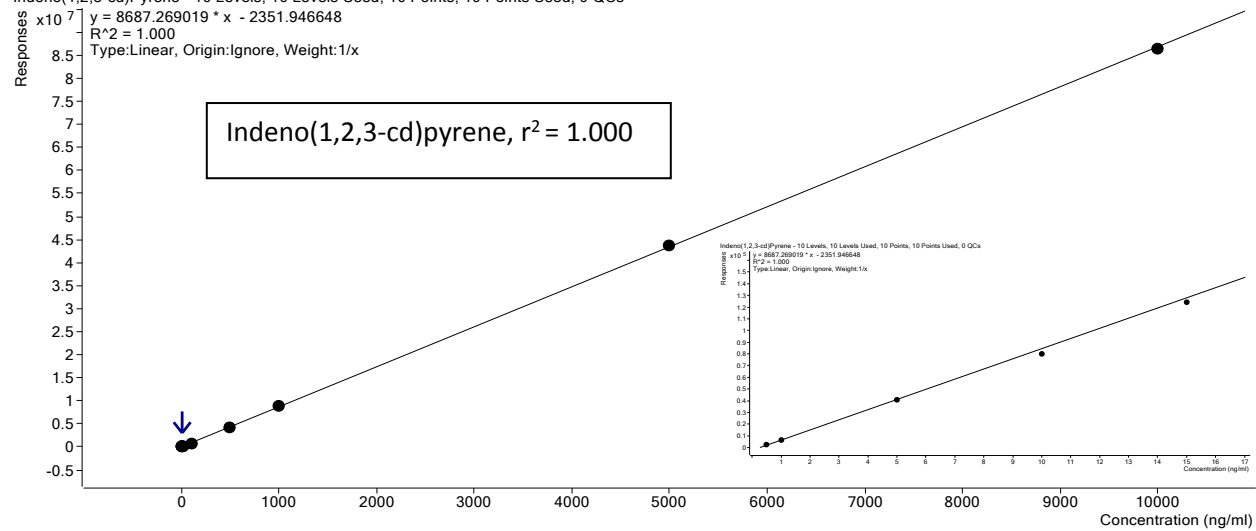


Indeno(1,2,3-cd)Pyrene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$$y = 8687.269019 \cdot x - 2351.946648$$

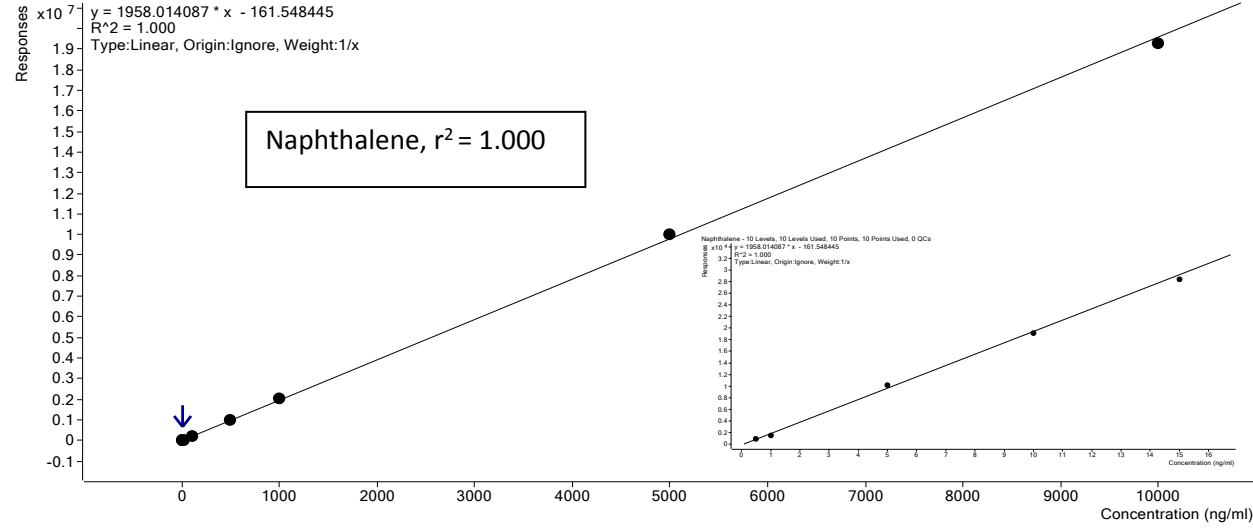
$R^2 = 1.000$

Type:Linear, Origin:Ignore, Weight:1/x



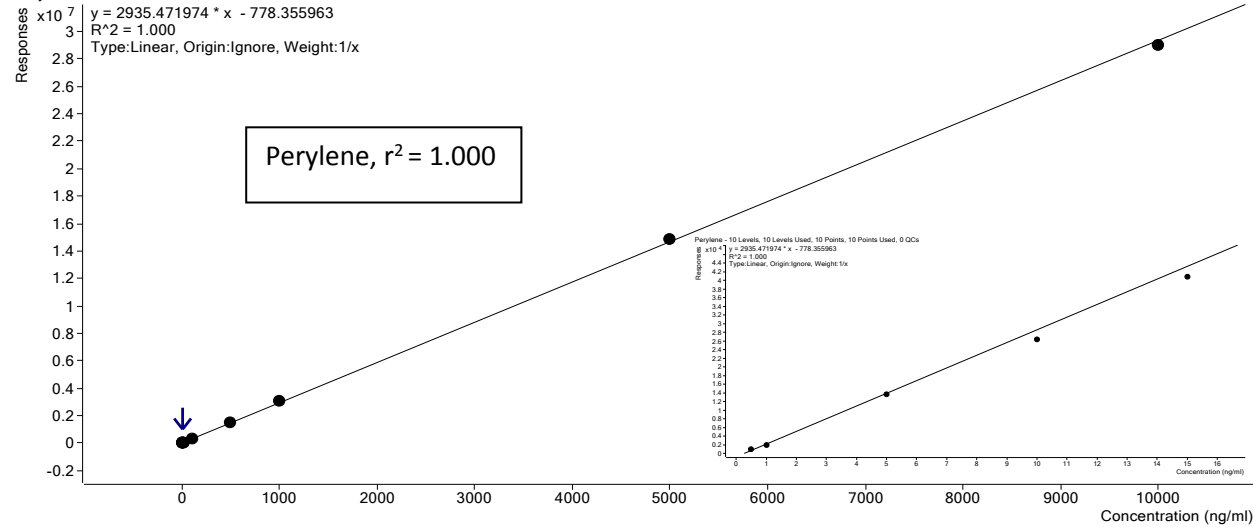
Naphthalene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 1958.014087 * x - 161.548445$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x

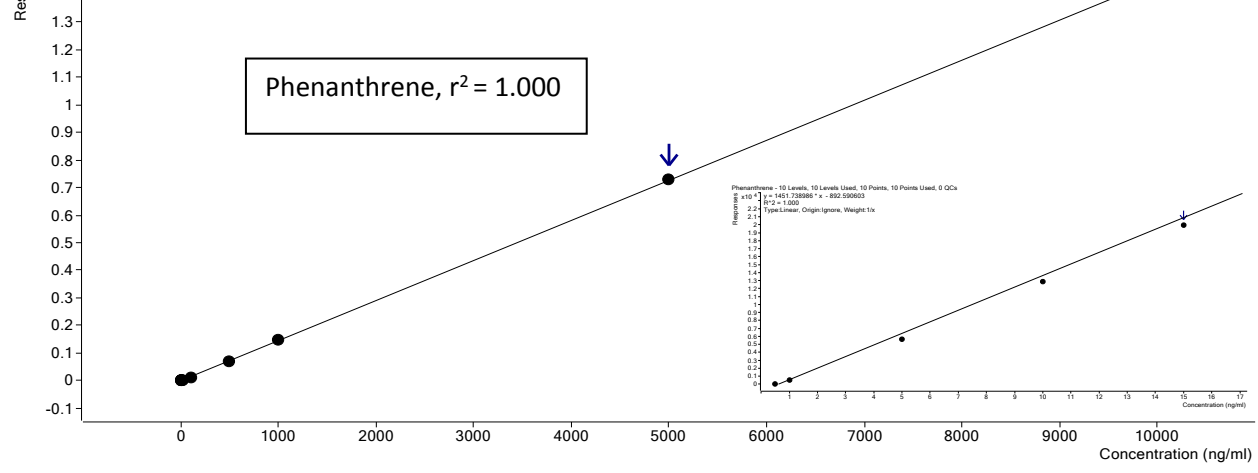


Perylene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs

$y = 2935.471974 * x - 778.355963$
 $R^2 = 1.000$
Type:Linear, Origin:Ignore, Weight:1/x



Phenanthrene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs
 $y = 1451.738986 * x - 892.590603$
 $R^2 = 1.000$
 Type:Linear, Origin:Ignore, Weight:1/x



Pyrene - 10 Levels, 10 Levels Used, 10 Points, 10 Points Used, 0 QCs
 $y = 1645.205386 * x - 412.728794$
 $R^2 = 1.000$
 Type:Linear, Origin:Ignore, Weight:1/x

