

Supporting Information

**Validation Studies of Thermal Extraction-GC/MS Applied to Source Emissions Aerosols: 1.
Semivolatile Analyte-Nonvolatile Matrix Interactions**

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Table S1. Calibration data for the TE/GC/MS method.

Internal Standard	Analyte	Class	Linear Range (ng)	r ²	MDL (ng)	RSD (%)	EQL (ng)
Dodecane-d26	Decane	Alkane	2.00 - 8.00	0.974	0.187	2.9	0.933
	Undecane	Alkane	2.00 - 8.00	0.976	0.064	10.0	0.322
	Dodecane	Alkane	2.00 - 8.00	0.971	0.044	6.8	0.219
	Tridecane	Alkane	2.00 - 8.00	0.974	0.051	7.9	0.254
Hexadecane-d34	Tetradecane	Alkane	2.00 - 8.00	0.967	0.040	6.2	0.200
	Pentadecane	Alkane	2.00 - 8.00	0.923	0.051	8.0	0.257
	Hexadecane	Alkane	2.00 - 8.00	0.984	0.064	9.9	0.319
	Heptadecane	Alkane	2.00 - 8.00	0.976	0.124	19.2	0.618
	Octylcyclohexane	Cyclic	2.00 - 9.52	1.000	0.030	9.5	0.149
	Decylcyclohexane	Cyclic	2.00 - 9.52	1.000	0.048	15.3	0.240
	Norpristane	Branched Alkane	2.00 - 9.52	1.000	0.048	12.7	0.238
	Pristane	Branched Alkane	2.00 - 9.52	1.000	0.597	12.7	2.500
	Phytane	Branched Alkane	2.00 - 9.52	1.000	0.068	18.2	0.341
Eicosane-d42	Octadecane	Alkane	2.00 - 8.00	0.983	0.144	22.4	0.721
	Eicosane	Alkane	2.00 - 8.00	0.977	0.116	18.0	0.579
	2-Methylnonadecane	Branched Alkane	1.96 - 2.35	0.989	0.020	6.6	0.102
	3-Methylnonadecane	Branched Alkane	1.96 - 2.35	1.000	0.010	3.5	0.054
	1-Octadecene	Alkene	3.83 - 15.32	0.978	0.304	25.3	1.521
	Tridecylcyclohexane	Cyclohexane	2.00 - 9.52	1.000	0.012	3.9	0.061
4,4'-Dimethoxybenzophenone-d8	Dibutylphthalate	Phthalate	4.00 - 19.05	0.996	0.055	8.7	0.273
	Butylbenzylphthalate	Phthalate	4.00 - 19.05	0.999	0.035	5.5	0.173
	Bis-2-Ethylhexylphthalate	Phthalate	4.00 - 19.05	0.999	0.053	8.4	0.264
	Dioctylphthalate	Phthalate	4.00 - 19.05	0.995	0.102	16.3	0.512
Octacosane-d58	Tetracosane	Alkane	2.00 - 8.00	0.995	1.132	175.9	5.661
	Octacosane	Alkane	2.00 - 8.00	0.955	0.335	5.2	1.674
	Squalane	Alkane	2.00 - 8.00	0.968	0.164	12.6	0.819
	Squalene	Alkene	2.00 - 8.00	0.997	0.089	11.3	0.443
	Nonadecylcyclohexane	Cyclohexane	2.00 - 9.52	0.999	0.039	12.5	0.196
Chrysene-d12	Fluoranthene	PAH	0.80 - 3.81	0.998	0.022	14.6	0.110
	Pyrene	PAH	0.40 - 1.90	0.995	0.021	28.6	0.107
	Chrysene	PAH	0.40 - 1.90	1.000	0.004	5.4	0.020
	Benzo[a]anthracene	PAH	0.40 - 1.90	1.000	0.007	9.1	0.036
	Benzo[k]fluoranthene	PAH	0.40 - 1.90	0.992	0.143	19.1	0.716
	Benzo[b]fluoranthene	PAH	0.80 - 3.81	0.999	0.327	21.8	1.635
	Benzo[a]pyrene	PAH	0.40 - 1.90	0.981	0.113	15.0	0.563
	Methylfluoranthene	PAH	0.10 - 0.40	0.987	0.067	41.8	0.334
	Retene	PAH	0.49 - 1.96	0.979	0.500	10.0	2.500
	1-Methylchrysene	PAH	0.10 - 0.40	0.959	0.054	21.3	0.270
	Anthraquinone	Oxy-PAH	1.18 - 4.72	0.984	0.155	32.5	0.774
	Naphthalic Anhydride	Oxy-PAH	2.04 - 8.16	0.976	0.128	17.2	0.641
	Indeno[1,2,3-cd]pyrene	PAH	0.40 - 1.90	1.000	0.050	6.6	0.248
	Dibenzo[ah]anthracene	PAH	0.80 - 3.81	0.999	0.140	9.3	0.698
Dibenzo[ah]anthracene-d14	Benzo[ghi]perylene	PAH	0.80 - 3.81	1.000	0.234	15.6	1.170
	Coronene	PAH	0.62 - 2.38	0.997	0.056	6.0	0.281

(Table S1. cont.)

Internal Standard	Analyte	Class	Linear Range (ng)	r ²	MDL (ng)	RSD (%)	EQL (ng)
Acenaphthene-d10	Naphthalene	PAH	4.00 - 19.05	1.000	0.043	11.4	0.214
	2-Methylnaphthalene	PAH	4.48 - 23.05	0.998	0.038	8.4	0.191
	1-Methylnaphthalene	PAH	4.84 - 21.33	1.000	0.027	6.4	0.134
	2,6-Dimethylnaphthalene	PAH	3.84 - 18.29	1.000	0.027	7.6	0.137
	Acenaphthene	PAH	4.00 - 19.05	1.000	0.004	1.1	0.021
	Fluorene	PAH	0.80 - 3.81	1.000	0.008	5.3	0.040
	1-Methylfluorene	PAH	2.00 - 9.50	0.999	0.042	11.1	0.208
	Phenanthrene	PAH	0.40 - 1.90	1.000	0.011	14.6	0.055
	Anthracene	PAH	0.40 - 1.90	1.000	0.011	15.0	0.056
	9-Methylanthracene	PAH	3.92 - 18.67	1.000	0.036	9.9	0.182
	9H-Fluoren-9-one	Oxy-PAH	2.17 - 8.68	0.982	0.228	33.5	1.141
	Dimethylphthalate	Phthalate	4.80 - 19.05	1.000	0.046	14.5	0.228
	Diethylphthalate	Phthalate	4.80 - 19.05	0.999	0.066	21.1	0.331
$\alpha\alpha\alpha$ -20R-cholestane-d4	$\alpha\beta\beta$ -20R-C ₂₇ -cholestane	sterane	0.2 - 0.95	0.991	0.020	5.4	0.101
	$\beta\alpha\alpha$ -20R-C ₂₇ -cholestane	sterane	0.2 - 0.95	0.989	0.011	2.8	0.053
	$\alpha\alpha\alpha$ -20S-C ₂₇ -cholestane	sterane	0.2 - 0.95	0.991	0.023	6.1	0.114
	$\alpha\alpha\alpha$ -20R-C ₂₇ -cholestane	sterane	0.2 - 0.95	0.979	0.024	6.5	0.122
	$\alpha\beta\beta$ -20R-C ₂₈ -methylcholestane	sterane	0.2 - 0.95	0.983	0.016	4.2	0.079
	$\alpha\beta\beta$ -20R-C ₂₉ -ethylcholestane	sterane	0.2 - 0.95	0.972	0.063	16.8	0.315
	17 α (H)-22,29,30-trisnorhopane	sterane	0.2 - 0.95	0.999	0.021	5.6	0.105

Table S2. Mean value recoveries (ng) of triplicate injections of the mid-level concentration standard for each of the matrices investigated. The relative standard deviation for each mean is given in parenthesis.

	Spiked	ET	QF	AF	WTC	DE	JE
<i>n</i> -Alkanes							
Decane	4.00	3.2 (8)	3.0 (16)	3.2 (19)	2.9 (11)	3.0 (18)	2.9 (6)
Undecane	4.00	3.3 (11)	3.2 (15)	3.3 (15)	3.1 (9)	3.3 (10)	3.0 (5)
Dodecane	4.00	3.4 (9)	3.3 (9)	3.4 (13)	3.2 (4)	3.4 (5)	3.0 (4)
Tridecane	4.00	3.7 (3)	3.26 (1)	3.4 (13)	3.12 (3)	3.48 (1)	3.0 (6)
Tetradecane	4.00	3.8 (16)	3.8 (8)	3.9 (11)	3.8 (6)	3.8 (4)	3.5 (5)
Pentadecane	4.00	3.3 (6)	3.22 (1)	3.4 (8)	3.1 (8)	3.5 (3)	2.79 (2)
Hexadecane	4.00	3.7 (4)	3.58 (1)	3.8 (5)	3.5 (7)	3.8 (3)	3.2 (3)
Heptadecane	4.00	3.5 (6)	3.45 (1)	3.7 (7)	3.4 (9)	3.8 (3)	3.1 (3)
Octadecane	4.00	3.6 (7)	3.53 (1)	3.8 (5)	3.5 (6)	3.8 (3)	3.28 (2)
Eicosane	4.00	3.6 (6)	3.53 (2)	3.7 (4)	3.5 (5)	3.8 (3)	3.27 (3)
Tetracosane	4.00	3 (37)	2.6 (33)	3.0 (16)	2.5 (8)	3.0 (16)	2.62 (1)
Octacosane	4.00	3.1 (12)	4.1 (9)	3.5 (5)	3.6 (4)	4.6 (3)	2.9 (13)
Branched Alkanes							
Pristane	5.00	5.0 (3)	4.99 (1)	5.03 (2)	4.9 (4)	5.04 (1)	4.81 (0.8)
Norpristane	5.00	4.93 (1)	4.98 (1)	4.98 (1)	4.9 (2)	5.00 (1)	4.85 (0.7)
Phytane	5.00	5.1 (3)	5.0 (2)	5.12 (2)	5.0 (5)	5.11 (1)	4.83 (0.6)
Squalane	10.45	9.0 (8)	8.2 (5)	9.3 (5)	8.4 (4)	9 (13)	9.0 (1)
3-Methylnonadecane	0.98	0.86 (2)	1.04 (2)	0.97 (5)	0.96 (6)	0.96 (5)	0.85 (3)
2-Methynonadecane	0.98	0.83 (8)	0.90 (3)	0.90 (7)	0.87 (5)	1.06 (4)	0.81 (1)
PAH							
Naphthalene	10.00	10 (11)	12 (13)	12 (9)	12.4 (2)	11.41 (1)	11 (10)
2-Methylnaphthalene	11.20	11 (10)	13.0 (7)	12.4 (5)	13.2 (2)	12.42 (0.2)	13 (7)
1-Methylnaphthalene	12.10	13 (10)	15 (7)	13.8 (4)	14.6 (2)	13.93 (0.3)	14 (8)
2,6-Dimethylnaphthalene	9.60	9.6 (2)	9.81 (1)	9.70 (0.4)	9.75 (0.6)	9.63 (1)	9.49 (1)
Acenaphthene	10.00	10.00 (1)	9.88 (0.8)	10.01 (0.5)	9.9 (1)	10.00 (0.6)	9.83 (0.3)
Fluorene	2.00	1.9 (10)	1.80 (4)	1.87 (2)	1.81 (2)	1.94 (1)	1.75 (4)
1-Methylfluorene	5.00	4.8 (10)	4.6 (3)	4.8 (3)	4.6 (6)	4.92 (1)	4.4 (3)
Phenanthrene	1.00	1.0 (10)	0.92 (3)	0.98 (4)	0.92 (7)	0.98 (0.6)	0.85 (3)
Anthracene	1.00	0.97 (9)	0.92 (3)	0.98 (4)	0.93 (6)	0.99 (0.6)	0.85 (3)
9-Methylanthracene	9.80	9.7 (10)	9.3 (4)	9.7 (7)	9.3 (6)	9.63 (0.8)	8.5 (4)
Fluoranthene	2.00	2.1 (10)	2.03 (4)	2.05 (3)	2.1 (5)	2.1 (9)	2.4 (4)
Pyrene	1.20	1.2 (11)	1.09 (5)	1.14 (3)	1.11 (6)	1.2 (9)	1.22 (3)
Chrysene	1.00	1.01 (2)	1.00 (1)	1.01 (0.6)	1.01 (0.6)	1.03 (2)	1.00 (2)
Benzo[a]anthracene	1.00	0.98 (0.6)	1.01 (1)	0.98 (0.6)	0.99 (1)	1.00 (2)	0.99 (2)
Benzo[k]fluoranthene	1.00	1.0 (32)	1.0 (18)	0.91 (10)	0.90 (1)	0.98 (9)	0.69 (6)
Benzo[b]fluoranthene	2.00	1.8 (39)	2.0 (23)	1.7 (13)	1.77 (2)	1.9 (13)	1.2 (10)
Benzo[a]pyrene	2.96	2.4 (39)	2.6 (22)	2.3 (19)	2.3 (5)	2.9 (9)	1.6 (6)
Indeno[1,2,3- <i>c,d</i>]pyrene	1.00	0.97 (10)	0.92 (2)	1.0 (14)	0.94 (6)	1.8 (12)	0.91 (5)
Dibenzo[<i>ah</i>]anthracene	2.00	2.03 (4)	2.00 (0.7)	2.2 (10)	2.09 (4)	3.4 (7)	1.9 (6)
Benzo[<i>ghi</i>]perylene	2.00	1.9 (10)	1.65 (0.9)	2.0 (18)	1.8 (16)	4.0 (17)	1.66 (0.7)
Coronene	1.25	1.3 (9)	1.2 (10)	1.26 (4)	1.21 (2)	0.9 (13)	1.12 (4)
1-Methylchrysene	0.20	0.16 (16)	0.16 (19)	0.16 (16)	0.14 (11)	0.17 (12)	0.12 (8)
Methylfluoranthene	0.20	0.18 (14)	0.17 (5)	0.18 (7)	0.17 (11)	0.20 (10)	0.18 (0)
Retene	0.98	0.9 (17)	0.79 (8)	0.87 (4)	0.82 (9)	0.9 (11)	0.85 (4)
Oxy-PAH							
Anthraquinone	2.36	2.1 (14)	1.95 (5)	2.15 (3)	2.0 (11)	1.4 (12)	2.09 (1)
Naphthalic Anhydride	4.43	3.4 (7)	3.2 (6)	3.6 (17)	3.2 (11)	4.4 (12)	2.8 (3)

Table S2 (cont.)								
9H-Fluoren-9-one	4.08	3.4 (9)	3.3 (6)	3.2 (6)	3.4 (14)	3.2 (5)	2.80 (6)	
Cyclohexanes								
Octylcyclohexane	5.00	5.2 (10)	5.5 (4)	5.3 (4)	5.6 (2)	5.07 (0.6)	5.4 (2)	
Decylcyclohexane	5.00	5.0 (2)	4.94 (1)	5.02 (0.4)	4.9 (2)	5.02 (0.3)	4.80 (0.3)	
Tridecylcyclohexane	5.00	4.89 (0.3)	4.83 (1)	4.91 (1)	4.80 (1)	4.86 (2)	4.77 (0.7)	
Nonadecylcyclohexane	5.00	4.5 (20)	3.6 (8)	4.2 (5)	3.7 (5)	3.9 (15)	4.1 (3)	
Cholestanes								
$\alpha\beta\beta$ -20R-C ₂₇ -cholestane	0.50	0.70 (6)	0.67 (1)	0.67 (5)	0.69 (4)	0.74 (6)	0.66 (3)	
$\beta\alpha\alpha$ -20R-C ₂₇ -cholestane	0.50	0.70 (7)	0.66 (4)	0.68 (5)	0.68 (4)	0.73 (5)	0.66 (3)	
$\alpha\alpha\alpha$ -20S-C ₂₇ -cholestane	0.50	0.70 (8)	0.65 (3)	0.67 (2)	0.68 (5)	0.75 (7)	0.67 (3)	
$\alpha\alpha\alpha$ -20R-C ₂₇ -cholestane	0.50	0.71 (2)	0.63 (3)	0.73 (3)	0.66 (5)	0.82 (5)	0.70 (6)	
$\alpha\beta\beta$ -20R-C ₂₈ -methylcholestane	0.50	0.71 (7)	0.79 (3)	0.74 (5)	0.79 (5)	0.85 (2)	0.69 (7)	
$\alpha\beta\beta$ -20R-C ₂₉ -ethylcholestane	0.50	0.70 (6)	0.75 (8)	0.68 (1)	0.74 (7)	0.75 (6)	0.65 (4)	
17 α (H)-22,29,30-trisnorhopane	0.50	0.67 (4)	0.66 (5)	0.70 (5)	0.70 (7)	0.73 (2)	0.69 (4)	
Phthalates								
Bis-(2-ethylhexyl)phthalate	10.00	10 (13)	10.7 (6)	10.4 (8)	10.7 (0.2)	9.3 (7)	11.2 (3)	
Butylbenzylphthalate	10.00	10.5 (3)	9.7 (3)	10.32 (0.5)	10.3 (1)	7.9 (6)	9.7 (2)	
Diethylphthalate	10.00	10 (10)	10.0 (4)	10.2 (4)	9.9 (4)	11.1 (4)	9.3 (3)	
Dimethylphthalate	10.00	10 (12)	9.8 (5)	10.0 (3)	9.6 (5)	10.2 (1)	9.1 (4)	
Di-n-butylphthalate	10.00	11 (11)	10.0 (4)	10.4 (4)	10.0 (3)	9.2 (3)	12.0 (5)	
Di-n-octylphthalate	10.00	10 (37)	13 (17)	11 (15)	12.3 (3)	10 (20)	10.0 (5)	
Alkenes								
Squalene	8.28	5.0 (6)	1.3 (59)	5.2 (12)	2.7 (16)	7 (79)	3 (35)	
1-Octadecene	7.66	6.3 (8)	6.17 (1)	6.5 (6)	5.88 (5)	6.8 (5)	5.5 (2)	

Table S3. For each matrix and control experiments, the percentage of compounds by class which have relative standard deviations within 10% and 20% of their respective means.

		LVL 1		LVL 2		LVL 3	
		1: 1 dilution		1:2 dilution		1:5 dilution	
		<20%	<10%	<20%	<10%	<20%	<10%
ET	n-Alkanes	100	91.7	91.7	66.7	100	75.0
	Branched Alkanes	100	100	100	100	100	100
	Alkenes	100	100	100	100	100	100
	PAH's	95.8	58.3	95.8	58.3	100	75.0
	Oxy-PAH's	100	66.7	100	66.7	100	100
	Cyclohexanes	100	75.0	100	75.0	100	100
	Cholestanes	100	100	100	100	100	85.7
	Phthalates	83.3	50.0	83.3	16.7	100	100
QF	n-Alkanes	91.7	75.0	91.7	75.0	100	91.7
	Branched Alkanes	100	100	100	100	100	83.3
	Alkenes	100	50.0	50.0	50.0	100	100
	PAH's	91.7	66.7	91.7	79.2	100	91.7
	Oxy-PAH's	100	66.7	100	100	100	100
	Cyclohexanes	100	75.0	100	100	100	100
	Cholestanes	100	85.7	100	100	100	100
	Phthalates	83.3	83.3	100	83.3	100	83.3
AF	n-Alkanes	91.7	83.3	100	50.0	87.5	75.0
	Branched Alkanes	100	66.7	100	100	100	83.3
	Alkenes	100	100	100	50.0	100	50.0
	PAH's	87.5	75.0	100	79.2	87.5	75.0
	Oxy-PAH's	100	100	100	66.7	100	100
	Cyclohexanes	75.0	75.0	100	100	100	75.0
	Cholestanes	100	85.7	100	100	100	71.4
	Phthalates	83.3	83.3	100	83.3	83.3	83.3
WTC	n-Alkanes	91.7	91.7	100	91.7	95.8	75.0
	Branched Alkanes	100	83.3	100	100	100	100
	Alkenes	50.0	50.0	100	50.0	50.0	50.0
	PAH's	95.8	62.5	100	87.5	95.8	75.0
	Oxy-PAH's	100	66.7	100	0	100	100
	Cyclohexanes	100	75.0	100	100	100	100
	Cholestanes	100	100	100	100	100	100
	Phthalates	83.3	83.3	100	100	100	83.3
DE	n-Alkanes	100	100	100	75.0	79.2	66.7
	Branched Alkanes	100	100	100	83.3	100	100
	Alkenes	50.0	50.0	50.0	50.0	50.0	50.0
	PAH's	95.8	91.7	100	75.0	79.2	66.7
	Oxy-PAH's	100	100	100	33.3	100	100
	Cyclohexanes	100	100	100	75.0	100	75.0
	Cholestanes	100	100	100	100	100	85.7
	Phthalates	100	83.3	83.3	83.3	83.3	50.0
JE	n-Alkanes	100	91.7	100	100	87.5	70.8
	Branched Alkanes	100	100	100	100	100	100
	Alkenes	100	50.0	50.0	50.0	100	100
	PAH's	95.8	83.3	100	100	87.5	70.8
	Oxy-PAH's	100	100	100	100	100	100
	Cyclohexanes	100	75.0	100	100	100	100
	Cholestanes	100	100	100	100	100	85.7
	Phthalates	83.3	83.3	100	100	100	100

Table S4. The complete list of organic compounds for which the *t*-test null hypothesis is rejected at $\alpha = 0.05$. Compounds listed in bold type also had means greater than 20% different than those of the empty thermal desorption tube (See Table 2).

		DE	JE	WTC	AF	QF
LVL 1 (no dilution)	PAH	Benzo[ghi]perylene Coronene Indeno[1,2,3-cd]pyrene Phenanthrene Anthracene Dibenzo[ah]anthracene Fluorene Methylfluoranthene 9-Methylanthracene	Benzo[a]pyrene Benzo[k]fluoranthene Fluoranthene 1-Methylnaphthalene 2-Methylnaphthalene Fluorene Benzo[a]anthracene 2,6-Dimethylnaphthalene	Benzo[a]pyrene Benzo[k]fluoranthene Benzo[b]fluoranthene Methylchrysene Retene Methylfluoranthene Fluoranthene Pyrene 2,6-Dimethylnaphthalene Benzo[a]anthracene		Benzo[a]anthracene 2,6-Dimethylnaphthalene
	OxyPAH	Naphthalic Anhydride	9H-Fluorenone	Anthraquinone		Naphthalic Anhydride
	n-alkane	Dodecane, Tetradecane, Octacosane	Decane , Undecane, Dodecane, Pentadecane, Hexadecane, Heptadecane, Octadecane, Eicosane	Decane, Undecane, Dodecane, Heptadecane, Octadecane, Octacosane	Undecane, Dodecane, Tetradecane, Octacosane	Tetradecane, Pentadecane Octacosane
	Branched Alkane		Pristane, Norpristane Phytane	Pristane, Norpristane Phytane		
	Alkene		1-Octadecene	Squalene 1-Octadecene		
	Phthalate	Butylbenzylphthalate Bis-2-ethylhexylphthalate	Bis-2-ethylhexylphthalate Di-n-butylphthalate	Butylbenzylphthalate Di-n-butylphthalate	Bis-2-ethylhexylphthalate	
	Cholestane	Ethylcholestane Methylcholestane	17 α (H) 22,29,30- Trisnorhopane		$\alpha\beta\beta$ -20R-C ₂₇ -cholestane	$\alpha\alpha\alpha$ -20R-C ₂₇ -cholestane
	Cyclohexane	Decylcyclohexane	Decylcyclohexane Tridecylcyclohexane	Decylcyclohexane Tridecylcyclohexane		

LVL 2 (1:2 dilution)	Table S4 (cont.)	PAH	Benzo[ghi]perylene Coronene Dibenzo[ah]anthracene Indeno[1,2,3-cd]pyrene Methylchrysene Benzo[a]anthracene	Methylchrysene 1-Methylnaphthalene Phenanthrene 9-Methylantracene 2-Methylnaphthalene Methylfluoranthene Anthracene, Acenaphthalene	Naphthalene 1-Methylnaphthalene 2-Methylnaphthalene Acenaphthene		1-Methylnaphthalene 2-Methylnaphthalene Benzo[a]anthracene
		Oxy-PAH	Naphthalic Anhydride Anthraquinone	9H-Fluorenone			
		n-Alkane	Octacosane	Tridecane, Pentadecane Hexadecane, Heptadecane Octadecane, Eicosane	Tridecane		Tridecane, Octacosane
		Branched Alkane	2-Methylnonadecane 3-Methylnonadecane		3-Methylnonadecane	3-Methylnonadecane	3-Methylnonadecane
		Alkene		1-Octadecene			
		Phthalate	Butylbenzylphthalate Di-n-butylphthalate	Butylbenzylphthalate			Butylbenzylphthalate
		Cholestane	$\alpha\beta$ -20R-C ₂₇ -cholestane Methylcholestane		Methylcholestane		$\alpha\alpha\alpha$ -20R-C ₂₇ -cholestane Methylcholestane
		Cyclohexane		Decylcyclohexane Tridecylcyclohexane			Nonadecylcyclohexane

LVL 3 (1:5 dilution)	Table S4 (cont.)	PAH	Benzo[ghi]perylene Coronene Dibenzo[ah]anthracene Indeno[1,2,3-cd]pyrene Fluorene Methylfluoranthene Phenanthrene Anthracene 9-Methylanthracene Benzo[a]anthracene Chrysene	Benzo[b]fluoranthene Fluoranthene Methylchrysene Retene 2-Methylnaphthalene Fluorene Methylfluoranthene Phenanthrene Anthracene Benzo[a]anthracene Chrysene	Naphthalene Methylfluoranthene Fluorene Phenanthrene Anthracene 9-Methylanthracene	Fluorene Methylfluoranthene Phenanthrene Anthracene 9-Methylanthracene	Fluorene Methylfluoranthene Phenanthrene Anthracene 9-Methylanthracene
		Oxy-PAH	Naphthalic Anhydride 9H-Fluoren-9-one Anthraquinone	9H-Fluoren-9-one Naphthalic Anhydride	9H-Fluorenone	Naphthalic Anhydride 9H-Fluorenone	9H-Fluorenone
		n-Alkane	Tetradecane Dodecane, Pentadecane, Heptadecane, Octacosane	Dodecane, Tetradecane Pentadecane	Tridecane Dodecane, Tetradecane Pentadecane, Octacosane	Dodecane, Tetradecane Pentadecane	Dodecane, Pentadecane, Octacosane
		Branched Alkane	Squalane, Pristane Phytane, Norpristane	Squalane, Pristane Norpristane, Phytane	Pristane, Norpristane	Squalane, Norpristane	Squalane, Pristane Norpristane, Phytane
		Alkene	Squalene		Squalene		Squalene
		Phthalate	Butylbenzylphthalate Bis-2-ethylhexylphthalate Diethylphthalate Dimethylphthalate	Dioctylphthalate Di-n-butylphthalate Diethylphthalate Dimethylphthalate Butylbenzylphthalate	Diethylphthalate Dimethylphthalate	Diethylphthalate Dimethylphthalate	Diethylphthalate Dimethylphthalate
		Cholestane	$\alpha\beta$ -20R-C ₂₇ -cholestane	Ethylcholestane Methylcholestane	$\alpha\alpha\alpha$ -20R-C ₂₇ -cholestane $\alpha\beta\beta$ -20R-C ₂₇ -cholestane $\beta\alpha\alpha$ -20R-C ₂₇ -cholestane		$\alpha\alpha\alpha$ -20R-C ₂₇ -cholestane
		Cyclohexane	Octylcyclohexane Nonadecylcyclohexane Decylcyclohexane Tridecylcyclohexane	Octylcyclohexane Tridecylcyclohexane Nonadecylcyclohexane	Octylcyclohexane Tridecylcyclohexane	Octylcyclohexane	Tridecylcyclohexane

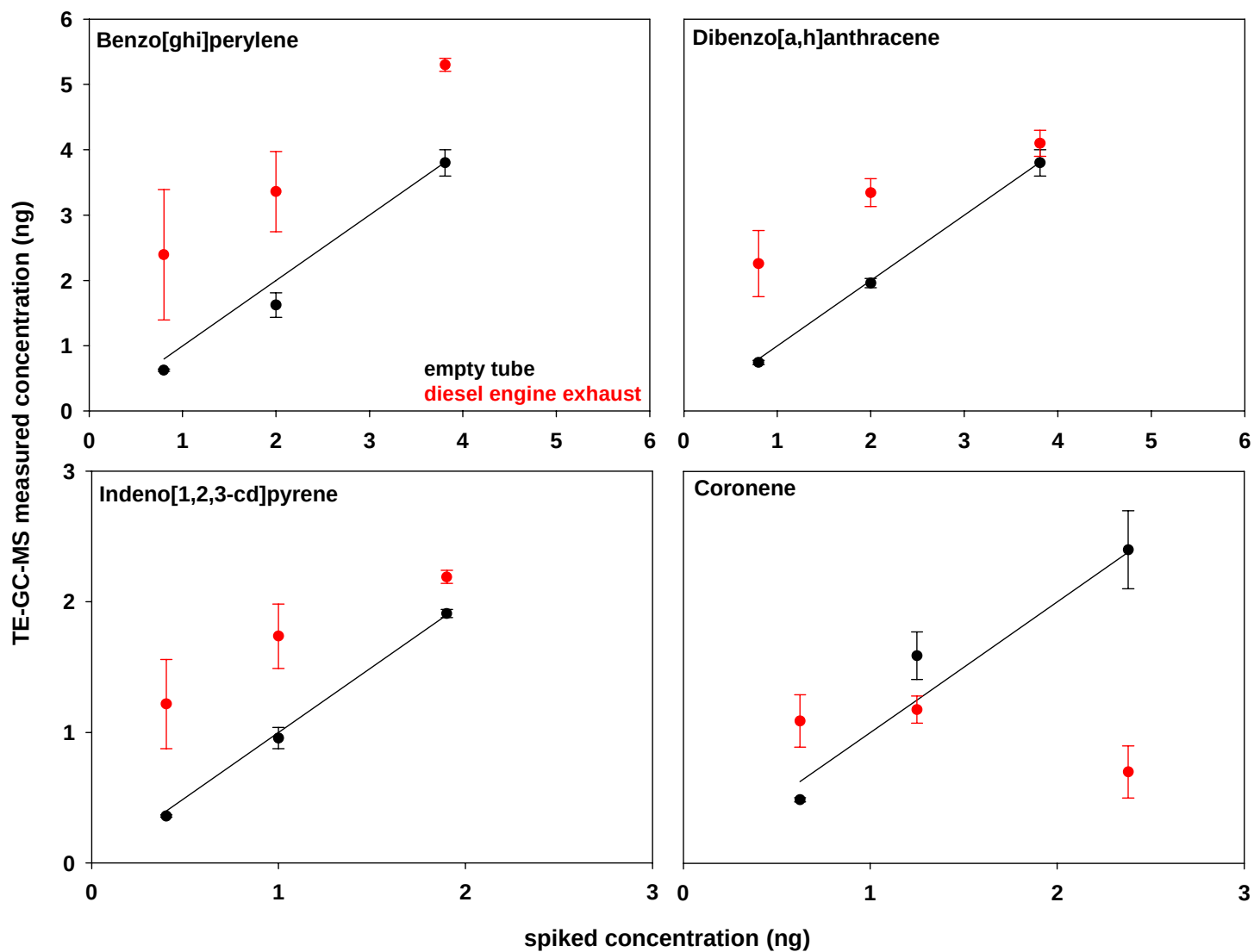


Figure S1. Representative six- and seven-member ring PAH that undergo substantial DE matrix bias.