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Table 1. List of Analytes and their Group Subsets

	conc.[a]	Chemical Properties[b]						
	ppb	α_{Kw}	bp(°C)	K_{ow}	BCF	K_{ao}[c]	α_{Ko} avg	α_{Ko} dev
volatile gases								
dichlorodifluoromethane	20	0.07	-30	144.5	7	10	3	2
trichlorofluoromethane	20	0.20	24	339.0	7	68	48	4
vinyl chloride	20	0.48	-13	4.0	7	2	8	4
chloroethane	20	1.01	12	26.9	7	27	60	9
chloromethane	20	1.37	-24	8.1	7	11	13	3
bromomethane	20	1.82	4	12.6	7	23	42	7
Volatiles								
1,1-dichloroethene	10	0.63	37	30.2	5	19	220	150
carbon tetrachloride	10	0.64	76.5	537.0	5	340	570	240
1,1-dichloropropene	10	0.88	104	37.2	5	33	320	80
1,1,1-trichloroethane	10	1.31	74	295.0	5	390	420	140
allyl chloride	10	1.34	45	26.9	5	36	47	18
2,2-dichloropropane	10	1.37	69	380.2	5	520	200	30
tetrachloroethene	10	1.43	121	339.0	5	480	6100	300
iodomethane	10	2.29	42	30.2	5	69	29	14
trans-1,2-dichloroethene	10	2.30	48	211.4	5	490	89	14
trichloroethene	10	2.34	87	339.0	5	790	2600	600
isopropylbenzene	10	2.75	152	4571.0	5	12600	9200	500
benzene	10	3.55	80	134.9	5	480	460	80
ethylbenzene	10	3.60	136	1413.0	5	5100	5000	340
toluene	10	3.88	111	490.0	5	1900	2100	170
m,p-xylenes	10	3.91	138	1479.1	5	5800	4500	200
1,1-dichloroethane	10	4.12	57	61.7	5	250	180	24
n-propylbenzene	10	2.43	159	4786.0	5	12000	11000	830
cis-1,2-dichloroethene	10	5.34	60	30.2	5	160	210	10
o-xylene	10	5.54	144	1318.3	5	7300	8200	160
chlorobenzene	10	6.07	132	691.8	5	4200	5700	130
chloroform	10	6.39	62	93.3	5	600	570	45
styrene	10	6.87	145	1445.0	5	9900	8500	150
bromobenzene	10	7.89	156	977.2	5	7700	12000	1000
methylene chloride	10	10.10	40	17.8	5	180	100	10
1,2-dichloropropane	10	10.90	96	190.6	5	2100	14000	370
1,1,1,2-tetrachloroethane	10	11.60	130.5	1096.0	5	13000	7700	270
bromodichloromethane	10	12.30	90	75.9	5	930	2900	1000
trans-1,3-dichloropropene	10	14.10	112	25.7	5	360	1900	90
bromochloromethane	10	15.40	68	25.7	5	400	470	90
1,2-dichloroethane	10	18.70	84	28.2	5	530	810	30
dibromochloromethane	10	19.20	120	123.0	5	2400	9300	1500
cis-1,3-dichloropropene	10	19.60	104	25.7	5	500	5600	4200
bromoform	10	17.39	150	199.5	5	3500	17000	1700

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dibromomethane	10	23.90	97	11.8	5	2800	1800	100
1,3-dichloropropane	10	24.90	120	95.5	5	2400	3400	400
1,1,2-trichloroethane	10	26.20	114	148.0	5	3900	3500	700
1,2-dibromoethane	10	26.70	132	39.8	5	1100	4900	200
1,1,2,2-tetrachloroethane	10	23.63	146	245.0	5	5800	23000	2400
cis-1,4-dichloro-2-butene	10	33.30	152	24.5	5	820	11000	460
1,2,3-trichloropropane	10	33.60	157	234.4	5	7900	14000	990
trans-1,4-dichloro-2-butene	10	33.80	156	24.5	5	830	14000	770
check surrogates								
Fluorobenzene	5	3.50	85	195	3	680	690	60
1,4-difluorobenzene	5	3.83	88.5	226	3	870	860	70
4-bromofluorobenzene	5	5.97	152	1350.0	3	8100	13000	1400
methylene chloride-d_6	5	11.10	40	17.8	3	200	98	15
1,2-dichloropropane-d_6	5	11.00	95	190.6	3	2100	98	15
1,1,2-trichloroethane-d_3	5	26.60	112	148.0	3	3900	3800	20
neutral semivolatiles								
n-butylbenzene	10	1.88	183	15849.0	5	30000	22000	4500
sec-butylbenzene	10	1.91	173	17378.0	5	33000	16000	2300
hexachlorobutadiene	10	2.08	215	60256.0	5	130000	38000	14000
p-isopropyltoluene	10	2.50	183	12589.0	5	31000	35000	8900
tert-butulbenzene	10	2.72	169	12882.0	5	35000	15000	1800
1,3,5-trimethylbenzene	10	3.75	165	2630.0	5	9900	15000	1700
2-chlorotoluene	10	4.04	159	2399.0	5	9700	13000	1500
1,2,4-trimethylbenzene	10	4.50	169	4266.0	5	19000	16000	2200
4-chlorotoluene	10	4.78	162	2399.0	5	11000	14000	1500
1,3-dichlorobenzene	10	5.72	173	2399.0	5	14000	20000	3500
1,4-dichorobenzene	10	6.14	174	2455.0	5	15000	20000	3500
1,2,4-trichlorobenzene	10	7.33	214	9550.0	5	74000	39000	4500
1,2-dichlorobenzene	10	7.86	180	2399.0	5	19000	21000	3500
1,2,3-trichlorobenzene	10	11.30	218	13804.0	5	16000	46000	200
pentachloroethane	10	13.20	162	1120.0	5	15000	24000	6000
naphthalene	20	11.03	218	2344.0	7	26000	41000	2000
1,2-dibromo-3-chloropropane	10	38.90	196	426.6	5	17000	36000	7600
check surrogates								
decafluorobiphenyl	5	3.03	206	2253.0	3	6800	35000	8900
naphthalene-d_8	10	18.00	217	2344.0	89	42000	57000	24000
soluble volatiles								
diethyl ether	10	34.90	35	6.8	5	240	360	310
ethyl methacrylate	10	48.40	117	109.7	5	5300	2200	290
methyl methacrylate	10	71.40	101	24.0	5	1700	1200	88
methacrylonitrile	10	102.90	90	8.2	5	840	400	53
4-methyl-2-pentanone	20	119.90	117	12.3	7	1500	2000	180
2-hexanone	10	131.10	128	60.3	5	7900	2300	1100
acrylonitrile	10	161.00	78	1.8	5	290	190	49
2-butanone	10	770.00	80	1.8	5	1400	710	700

propionitrile	10	1420.00	97	1.4	5	2000	680	120
1,4-dioxane	10	5750.00	101	0.5	5	2900	1700	210
check surrogates								
acetophenone-d_5	20	161.00	202	38.0	7	6100	28000	1800
nitromethane-d_3	5	510.00	101	0.5	3	260	14	23
acetone-d_6	50	600.00	57	0.6	11	350	230	17
basic semivolatiles								
n-nitrosodimethylamine	67	129.00	154	0.7	13	39000	5300	3700
n-nitroso-methyl-ethylamine	67	1900.00	165	2.3	13	44000	7000	3900
n-nitrosodi-n-propylamine	67	2400.00	206	1.2	13	2900	20000	5100
n-nitrosodiethylamine	67	4900.00	177	7.9	13	39000	11000	3000
aniline	10	13700.00	184	7.9	5	108000	30000	14000
o-toluidine	67	15200.00	200	36.1	13	550000	46000	24000
marginal analytes								
2-methylnaphthalene	67	67.00	245	10700	13	720000	130000	150000
2-picoline	10	6800.00	129	21.5	5	150000	20000	1900
pyridine	10	13100.00	116	4.7	3	62000	16000	8500
n-nitrosodibutylamine	67	21000.00	240	239.9	13	5000000	64000	91000
check surrogates								
nitrobenzene-d_5	5	87.50	210	69.2	3	6100	38000	6700
surrogate correction compounds								
hexafluorobenzene	5	0.86	81.5	79.0	3	68	130	16
pentafluorobenzene	5	1.51	85	51.9	3	78	350	170
benzene-d_6	10	3.92	79	135.0	5	530	500	60
toluene-d_8	5	4.28	111	490.0	3	2100	2200	110
o-xylene-d_{10}	5	6.14	143	1318.3	3	8100	8400	340
chlorobenzene-d_5	5	6.27	131	692.0	3	4300	5800	280
1,2,4-trichlorobenzene-d_3	5	7.88	213	9550.0	3	75000	41000	6800
bromobenzene-d_5	5	7.93	155	977.0	3	7700	12000	1000
1,2-dichlorobenzene-d_4	5	8.03	181	2399.0	3	19000	22000	4000
1,2-dichloroethane-d_4	5	20.00	84	28.2	3	560	810	70
1,2-dibromoethane-d_4	5	26.00	131	39.8	3	1040	5000	180
diethyl ether-d_{10}	5	32.50	35	6.8	3	220	105	130
1-methylnaphthalene-d_{10}	20	67.00	241	10700	7	720000	370000	490000
ethyl acetate-C^{13}	50	150.00	77	5.0	11	750	330	50
tetrahydrofuran-d_8	5	355.00	66	6.6	3	2300	380	60
1,4-dioxane-d_8	50	5800.00	101	0.5	11	2900	1600	160
pyridine-d_5	50	15000.00	115	4.7	11	70000	13000	9000

[a]Concentration of analytes used in this study for 10 g samples. The concentration of analytes in the 1 g samples were 10 times more concentrated.

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[b]The chemical property values were obtained from the following references: relative volatilities (α_{Kw}, ref. 5), boiling points (bp, ref. 10), the octanol-water partition coefficients (K_{oa}) were from reference 10 or calculated using Leo's fragment constant approach (ref. 11), and the bioconcentration factors (BCF) were calculated using the Neely formula (Ref. 6).
[c]The octanol-air partition coefficients (K_{oa}) were calculated using the relationships of fugacity constants (ref. 9). The experimental K_{oa} were obtained by averaging six sets of data. The deviation is 1 sigma.

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Table 2. Results for Surrogate Correction Model 1[a]

	relative response[b]		recovery[c]			MDL[e]		
group[f]	avg	dev	avg	dev	Surr[d] avg	avg	dev	median
volatile gases	0.84	0.08	101%	6%	18%	5.0	0.9	4.9
volatiles	0.52	0.16	92%	18%	8%	3.7	9.4	1.6
neutral semivolatiles	0.26	0.07	104%	11%	11%	4.3	7.3	1.9
soluble volatiles	0.81	0.23	109%	19%	5%	6.7	7.1	3.0
basic semivolatiles	1.45	0.61	327%	214%	24%	68.2	72.4	48.4
marginals	0.84	0.56	111%	70%	103%	62.7	72.5	43.0

[a]One g tissue samples (triplicates of 7 composites and canned tuna) were sonication spiked with an overnight equilibration period (>1000 min) prior to analyses. The analyte concentrations are 10 times those listed in Table 1.
[b]Relative response ratio is the response of analytes from the sample divided by the analyte response from the aqueous standard. The deviation is 1 sigma.
[c]Recovery is the measured analyte relative response divided by the predicted surrogate-corrected relative response. The diviation is 1 sigma.
[d]Average predicted surrogate-correction precision.
[e]Method detection limits are calculated as 3 times the precision for 21 determinations of analytes at concentrations approximately 3 times their estimated MDLs. The average, deviation, and median are of the individual analytes withing the group.
[f]Analyte contained in groupings are identified in Table 1.

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Table 3. Matrix Surrogates and Their Respective Ranges

range		surrogate pairs[a]	
type	values	first surrogates	second surrogates
α_{Kw}-values	<25	methylene chloride-d_2	1,2-dichloroethane-d_4
		pentafluorobenzene	1,2-dibromoethane-d_4
	25 to 200	1,2-dichloroethane-d_4	ethyl acetate-2C^{13}
		1,2-dibromoethane-d_4	tetrahydrofuran-d_{10}
	>200	ethyl acetate-2C^{13}	1,4-dioxane-d_8
		tetrahydrofuran-d_{10}	pyridine-d_5
α_{Ko}-values	<500	hexafluorobenzene	benzene-d_6
			toluene-d_8
	500 to 5000	benzene-d_6	chlorobenzene-d_5
		toluene-d_8	*o*-xylene-d_{10}
	5000 to 10000	chlorobenzene-d_5	bromobenzene-d_5
		o-xylene-d_{10}	1,2-dichlorobenzene-d_4
	>10000	bromobenzene-d_5	1,2,4-trichlorobenzene-d_3
		1,2-dichlorobenzene-d_4	1-methylnaphthalene-d_{10}

[a]The surrogate pair combinations used in Model 2 were all combinations of one from the first surrogate column and one from the second surrogate column for each value range.

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Table 4. Results for Surrogate Correction Model 2[a]

	1 g tissue samples					10 g tissue samples							
	relative response[b]		recovery[c] (%)		Surr[d] (%)	relative response		recovery(%)		Surr (%)	MDL[e]		
group[f]	avg	dev	avg	dev	avg	avg	dev	avg	dev	avg	avg	dev	median
volatile gases	0.84	0.08	103%	14%	65%	0.49	0.20	86%	44%	27%	0.7	0.4	0.8
volatiles	0.52	0.16	96%	14%	24%	0.30	0.20	97%	27%	25%	0.4	0.8	0.2
neutral semivolatiles	0.26	0.07	110%	19%	17%	0.07	0.02	90%	16%	24%	0.5	0.8	0.3
soluble volatiles	0.81	0.23	101%	28%	53%	0.62	0.39	124%	64%	94%	0.5	0.5	0.2
basic semivolatiles	1.45	0.61	248%	68%	182%	0.48	0.19	87%	36%	84%	13.1	16.0	3.5
marginals	0.84	0.56	122%	46%	48%	0.29	0.21	100%	32%	93%	3.9	4.9	1.6

[a]Samples were vacuum spiked with an overnight equilibration period (>1000 min) prior to analyses. One g samples consisted of 7 composites and canned tuna. The 10 g samples were only of canned tuna. Analyte concentrations of 10 g samples are listed in Table 1. Concentrations of 1 g samples are 10 times the values listed in Table 1.

[b]Relative response ratio is the response of analytes from the sample divided by the analyte response from the aqueous standard. The deviation is 1 sigma.

[c]Recovery is the measured analyte relative response divided by the predicted surrogate-corrected relative response. The diviation is 1 sigma.

[d]Average predicted surrogate-correction precision.

[e]Method detection limits are calculated as 3 times the precision for quadruple determinations of analytes at concentrations approximately 3 times their estimated MDLs. The average, deviation, and median are of the individual analytes withing the group.

[f]Analyte contained in groupings are identified in Table 1.

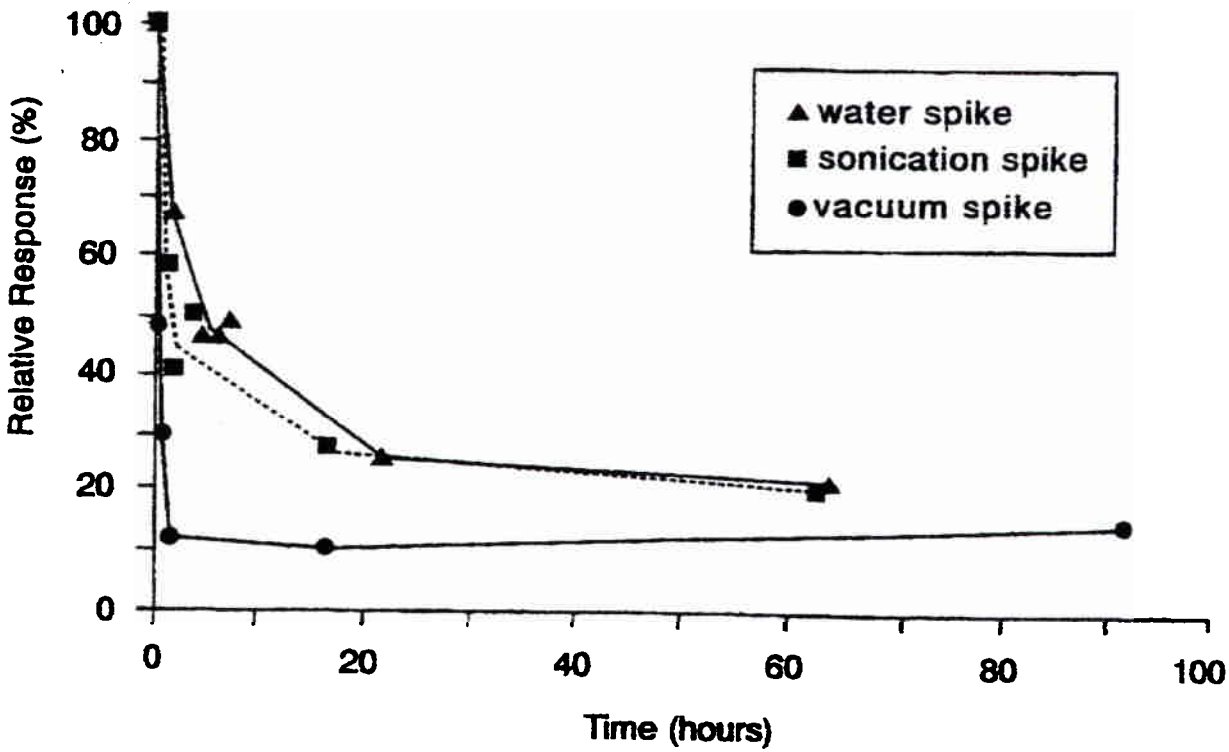

Figure 1. Relative response over equilibration times for naphthalene-d_8 and 1 g of tissue using the different spike techniques.