

US EPA ARCHIVE DOCUMENT

Supplementary Table 6. Comparison of Recoveries of Labelled Surrogates to unlabelled Analogs for Vacuum Spiked Tuna when the Unlabelled Analogs are Equilibrated an Additional 120 min.

compounds ^b	K _{oa} ^c	mol wt ^d	bp ^e	K _{ow} ^f	125 min ^a recovery ^g	146 min recovery	159 min recovery	178 min recovery	190 min recovery	211 min recovery	corr ^h
benzene	460	78	80	135	104%	96%	98%	94%	100%	97%	-0.491
1,2-Dichloroethane	810	98	84	28	98%	98%	99%	94%	99%	94%	-0.494
1,2-dichloropropane	2100	112	96	191	98%	95%	98%	97%	100%	95%	-0.137
dioxane	1700	88	101	1	108%	102%	116%	112%	112%	109%	0.299
toluene	2100	92	111	490	168%	161%	183%	169%	218%	186%	0.589
1,1,2-trichloroethane	3500	132	114	148	99%	96%	92%	90%	93%	97%	-0.311
pyridine	16000	79	116	5	103%	100%	104%	102%	103%	96%	-0.524
1,2-dibromoethane	4900	186	132	40	100%	93%	95%	93%	97%	93%	-0.553
chlorobenzene	5700	112	132	692	94%	84%	93%	92%	104%	103%	0.691
o-Xylene	8200	106	144	1318	95%	84%	97%	96%	114%	106%	0.705
bromobenzene	12000	156	156	977	88%	82%	86%	92%	103%	105%	0.861
1,2-dichlorobenzene	21000	146	180	2399	83%	83%	89%	100%	106%	109%	0.958
1,2,4-trichlorobenzene	39000	180	214	9550	66%	60%	83%	89%	133%	114%	0.855
naphthalene	41000	128	218	2344	82%	72%	95%	99%	123%	127%	0.911
methylnaphthalene	130000	142	245	10700	53%	58%	64%	66%	97%	89%	0.880
correlation all compounds ⁱ	0.457	0.322	0.739	0.544							
corr last seven compounds ^j	0.250	0.473	0.503	0.143							

^aPeriod of equilibration for surrogate compounds. Analog analytes were vacuum spiked for 120 min prior to the surrogate addition. Samples were 10 g aliquots of canned tuna with analyte concentrations as listed in Table 1.

^bList of surrogate-analytes that are analogs used for comparison.

^cExperimental values for relative volatility of analytes from organic phase.

^dMolecular weight of unlabelled analyte.

^eBoiling point of unlabelled analyte.

^fOctanol-water partition coefficient of unlabelled analyte.

^gResponse of surrogate (normalized to standard) to response of unlabelled analyte (normalized to standard) as a percent.

^hCorrelation of surrogate/unlabelled analyte response to surrogate vacuum spike equilibration time.

ⁱCorrelation of the time:recovery correlation to the compound chemical properties using all compound pairs.

^jCorrelation of the time:recovery correlation to compound properties for the last seven compounds.