Supplementary Table 2. Results for Surrogate Correction Models by Analyte[a]

	1g sample size													10g sample size				
	water standards[b]								tuna standards[c]					water standards				
	relative[d] response		Model 1 recovery[e]		surr[f]	Model 2 recovery		surr	relative response		Model 1 recovery		surr	relative response		Model 2 recovery		surr
compound	avg	dev	avg	dev	avg	avg	dev	avg	avg	dev	avg	dev	avg	avg	dev	avg	dev	avg
dichlorodifluoromethane	0.96	0.15	109%	22%	24%	117%	44%	26%	0.93	0.11	116%	17%	16%	0.62	0.10	73%	26%	12%
chloromethane	0.83	0.18	105%	16%	16%	104%	32%	59%	0.82	0.12	102%	13%	10%	0.57	0.06	119%	9%	46%
vinyl chloride	0.90	0.15	105%	20%	21%	124%	53%	84%	0.92	0.11	115%	15%	14%	0.56	0.07	149%	27%	74%
bromomethane	0.69	0.15	90%	19%	11%	83%	17%	43%	0.73	0.16	88%	18%	7%	0.05	0.01	10%	2%	3%
chloroethane	0.83	0.09	102%	21%	18%	96%	10%	39%	0.88	0.09	110%	17%	11%	0.61	0.07	95%	15%	22%
trichlorofluoromethane	0.85	0.11	97%	24%	21%	111%	51%	14%	1.00	0.09	125%	18%	16%	0.55	0.06	68%	26%	7%
diethyl ether-d_{10}	0.83	0.14	113%	9%	4%	117%	20%	81%	0.81	0.09	108%	9%	3%	0.58	0.03	92%	9%	61%
ether	0.77	0.12	104%	10%	4%	113%	19%	80%	0.80	0.10	106%	10%	3%	0.53	0.03	94%	6%	69%
acetone-d_6	0.36	0.06	41%	27%	0%	54%	26%	51%	0.97	0.16	149%	20%	1%	0.33	0.07	56%	12%	54%
1,1-dichloroethene	0.51	0.34	44%	54%	8%	65%	44%	23%	1.26	0.76	134%	31%	15%	0.85	0.19	158%	25%	36%
iodomethane	0.21	0.20	10%	101%	1%	23%	21%	8%	1.74	1.76	57%	129%	3%	0.00	0.00	0%	0%	0%
allyl chloride	0.53	0.21	55%	75%	9%	61%	22%	25%	1.02	0.49	96%	79%	9%	0.43	0.08	67%	14%	16%
methylene chloride-d_6	0.66	0.16	94%	18%	3%	84%	17%	40%	0.89	0.19	109%	19%	2%	0.55	0.07	95%	3%	27%
methylene chloride	0.52	0.14	74%	24%	2%	66%	13%	31%	0.75	0.15	91%	21%	2%	0.59	0.08	103%	3%	29%
acrylonitrile	0.56	0.13	64%	25%	0%	83%	22%	73%	0.50	0.15	75%	28%	0%	0.39	0.18	66%	29%	58%
trans-1,2-dichloroethene	0.58	0.15	77%	29%	7%	68%	14%	25%	0.72	0.19	84%	32%	5%	0.67	0.19	104%	22%	19%
nitromethane-d_3	0.99	0.38	121%	41%	3%	132%	35%	126%	0.85	0.27	133%	40%	2%	1.08	0.05	181%	11%	173%
1,1-dichloroethane	0.87	0.51	89%	74%	1%	103%	50%	21%	0.53	0.24	53%	40%	0%	0.92	0.42	141%	54%	18%
hexafluorobenzene	0.86	0.34	96%	28%	19%	97%	20%	18%	0.72	0.22	85%	22%	14%	0.83	0.23	114%	9%	9%
tetrahydrofuran-d_8	0.87	0.27	100%	0%	0%	112%	9%	82%	0.64	0.16	100%	0%	0%	0.58	0.02	101%	1%	76%
methacrylonitrile	0.74	0.18	103%	17%	5%	106%	11%	72%	0.72	0.13	100%	17%	5%	0.50	0.03	89%	3%	64%
2-butanone	1.08	0.25	122%	11%	2%	150%	41%	136%	0.96	0.18	149%	10%	1%	1.72	0.25	305%	46%	291%
propionitrile	0.94	0.28	113%	8%	5%	119%	23%	112%	0.76	0.19	120%	8%	3%	0.68	0.02	116%	4%	112%
ethyl acetate-2C^{13}	0.66	0.19	76%	17%	1%	93%	9%	70%	0.61	0.15	95%	18%	0%	0.58	0.03	100%	0%	79%
2,2-dichloropropane	0.73	0.10	94%	16%	14%	99%	37%	10%	0.87	0.11	108%	13%	10%	0.42	0.03	64%	18%	6%
cis-1,2-dichloroethene	0.67	0.09	102%	6%	3%	85%	6%	33%	0.82	0.10	100%	7%	2%	0.37	0.02	68%	5%	16%
chloroform	0.67	0.13	101%	6%	4%	107%	9%	22%	0.82	0.14	100%	7%	3%	0.35	0.02	121%	13%	25%
pentafluorobenzene	0.72	0.11	96%	16%	13%	93%	6%	31%	0.85	0.11	108%	11%	10%	0.39	0.03	79%	7%	25%
bromochloromethane	0.70	0.11	100%	5%	2%	100%	4%	45%	0.77	0.10	99%	5%	2%	0.43	0.02	98%	3%	46%
1,1,1-trichloroethane	0.72	0.12	91%	17%	14%	100%	20%	21%	0.91	0.13	113%	13%	10%	0.36	0.02	71%	12%	23%

1,1-dichloropropene	0.68	0.11	99%	20%	18%	86%	6%	32%	0.93	0.14	128%	15%	15%	0.32	0.02	66%	4%	21%
carbon tetrachloride	0.68	0.11	80%	22%	15%	111%	8%	10%	0.99	0.14	122%	17%	14%	0.22	0.04	77%	11%	11%
benzene-d_6	0.65	0.11	99%	1%	1%	90%	9%	25%	0.8	0.12	97%	1%	1%	0.33	0.02	73%	8%	30%
1,2-dichloroethane-d_4	0.70	0.12	100%	3%	2%	110%	4%	48%	0.75	0.1	100%	3%	2%	0.41	0.01	115%	5%	62%
1,2-dichloroethane	0.69	0.12	100%	3%	2%	110%	7%	47%	0.75	0.10	99%	3%	2%	0.42	0.02	125%	12%	63%
benzene	0.66	0.11	102%	3%	1%	92%	11%	24%	0.83	0.12	101%	3%	1%	0.36	0.02	76%	9%	29%
fluorobenzene	0.63	0.11	98%	2%	3%	102%	5%	13%	0.81	0.13	100%	1%	2%	0.30	0.01	106%	5%	17%
1,4-difluorobenzene	0.63	0.11	102%	1%	1%	103%	5%	13%	0.8	0.14	101%	1%	1%	0.30	0.02	107%	5%	17%
trichloroethene	0.49	0.10	71%	10%	6%	93%	6%	9%	0.68	0.13	86%	8%	5%	0.23	0.01	100%	6%	12%
1,2-dichloropropane-d_6	0.57	0.12	93%	2%	3%	98%	6%	12%	0.71	0.13	94%	2%	2%	0.32	0.01	122%	6%	19%
1,2-dichloropropane	0.57	0.12	93%	3%	3%	98%	5%	12%	0.69	0.13	93%	2%	2%	0.32	0.01	121%	5%	19%
methyl methacrylate	0.66	0.15	102%	13%	5%	105%	11%	51%	0.68	0.11	99%	13%	4%	0.36	0.02	90%	4%	56%
1,4-dioxane-d_8	1.38	0.27	121%	5%	23%	119%	10%	118%	0.87	0.17	111%	4%	12%	0.80	0.04	111%	4%	110%
bromodichloromethane	0.49	0.13	75%	9%	2%	90%	9%	22%	0.67	0.16	86%	11%	2%	0.21	0.01	87%	9%	23%
1,4-dioxane	1.31	0.28	115%	3%	22%	113%	6%	112%	0.84	0.17	108%	3%	11%	0.75	0.03	105%	3%	104%
dibromomethane	0.59	0.12	91%	4%	4%	85%	16%	58%	0.70	0.12	99%	4%	3%	0.34	0.01	56%	11%	47%
4-methyl-2-pentanone	0.74	0.19	128%	20%	8%	117%	10%	76%	0.69	0.14	108%	21%	6%	0.47	0.02	108%	3%	85%
trans-1,3-dichloropropene	0.39	0.17	61%	36%	2%	64%	25%	28%	0.49	0.21	61%	36%	2%	0.08	0.01	28%	8%	13%
toluene-d_8	0.52	0.13	98%	2%	4%	94%	5%	7%	0.72	0.17	99%	2%	2%	0.22	0.01	90%	1%	11%
toluene	0.53	0.13	101%	4%	4%	96%	7%	8%	0.72	0.18	98%	4%	2%	0.23	0.01	95%	3%	12%
pyridine-d_5	1.28	0.28	51%	25%	25%	52%	20%	50%	0.91	0.17	72%	16%	21%	0.65	0.11	71%	9%	70%
pyridine	1.25	0.29	61%	21%	27%	61%	19%	60%	0.90	0.18	81%	13%	20%	0.54	0.03	65%	4%	64%
cis-1,3-dichloropropene	0.40	0.15	61%	27%	2%	75%	21%	41%	0.50	0.18	66%	27%	2%	0.15	0.02	54%	8%	37%
ethyl methacrylate	0.55	0.12	100%	12%	5%	100%	15%	20%	0.60	0.10	95%	12%	4%	0.32	0.02	112%	6%	34%
n-nitrosodimethylamine	2.34	0.37	657%	28%	39%	384%	133%	374%	0.82	0.19	160%	30%	10%	0.71	0.09	130%	19%	129%
1,1,2-trichloroethane-d_3	0.47	0.12	80%	6%	4%	93%	6%	16%	0.62	0.14	93%	6%	3%	0.26	0.01	108%	2%	29%
2-hexanone	0.71	0.19	141%	23%	9%	125%	28%	39%	0.68	0.14	114%	23%	7%	0.49	0.02	156%	3%	68%
1,1,2-trichloroethane	0.46	0.12	82%	5%	4%	91%	6%	15%	0.61	0.14	93%	5%	3%	0.25	0.01	103%	2%	28%
tetrachloroethene	0.40	0.10	73%	16%	11%	99%	9%	12%	0.71	0.16	106%	12%	10%	0.12	0.00	81%	3%	7%
1,3-dichloropropane	0.52	0.12	99%	2%	5%	94%	10%	25%	0.61	0.12	97%	2%	3%	0.32	0.01	93%	13%	45%
dibromochloromethane	0.32	0.09	61%	11%	3%	82%	8%	20%	0.60	0.19	90%	19%	3%	0.15	0.01	90%	6%	32%
1,2-dibromoethane-d_4	0.45	0.12	99%	4%	6%	89%	4%	40%	0.57	0.13	98%	3%	4%	0.26	0.01	94%	1%	60%
2-picoline	1.53	0.43	163%	16%	38%	206%	37%	169%	0.91	0.17	131%	11%	16%	0.45	0.03	112%	4%	100%
1,2-dibromoethane	0.45	0.12	99%	4%	6%	86%	6%	37%	0.57	0.13	99%	4%	4%	0.26	0.01	89%	1%	54%
chlorobenzene-d_5	0.38	0.11	93%	4%	6%	94%	5%	8%	0.61	0.17	97%	4%	4%	0.15	0.01	98%	4%	5%
chlorobenzene	0.38	0.10	95%	3%	6%	94%	5%	8%	0.62	0.17	99%	3%	4%	0.14	0.01	95%	3%	5%

1,1,1,2-tetrachloroethane	0.38	0.11	88%	4%	5%	101%	3%	6%	0.59	0.17	95%	5%	3%	0.14	0.01	106%	1%	4%
ethylbenzene	0.43	0.12	111%	7%	4%	97%	5%	7%	0.69	0.19	110%	7%	2%	0.14	0.00	82%	1%	7%
n-nitroso-methyl-ethylamine	2.08	0.30	516%	31%	31%	289%	111%	269%	0.82	0.16	182%	27%	7%	0.65	0.07	115%	13%	112%
m,p-xylenes	0.40	0.11	107%	6%	3%	88%	4%	6%	0.66	0.18	107%	6%	2%	0.14	0.00	75%	1%	6%
styrene	0.33	0.09	94%	3%	4%	92%	3%	5%	0.55	0.15	96%	2%	3%	0.12	0.01	89%	4%	3%
o-xylene-d_{10}	0.36	0.11	101%	3%	5%	101%	4%	5%	0.59	0.17	100%	4%	3%	0.13	0.00	98%	1%	3%
o-xylene	0.36	0.10	102%	4%	4%	99%	3%	5%	0.59	0.16	101%	4%	3%	0.12	0.01	95%	2%	3%
isopropylbenzene	0.39	0.11	116%	15%	8%	114%	10%	5%	0.70	0.19	124%	15%	6%	0.12	0.01	93%	2%	1%
bromoform	0.20	0.08	53%	30%	2%	70%	22%	18%	0.70	0.31	118%	38%	4%	0.10	0.02	69%	14%	33%
cis-1,4-dichloro-2-butene	0.11	0.10	5%	134%	0%	25%	22%	15%	0.15	0.14	4%	134%	0%	0.01	0.00	2%	1%	2%
n-nitrosodiethylamine	1.64	0.21	356%	31%	62%	203%	55%	182%	0.85	0.14	168%	28%	18%	0.63	0.05	119%	7%	113%
1,1,2,2-tetrachloroethane	0.20	0.13	37%	62%	2%	74%	46%	18%	1.31	1.00	144%	72%	5%	0.04	0.01	35%	8%	14%
4-bromofluorobenzene	0.29	0.08	92%	4%	4%	112%	8%	16%	0.53	0.14	97%	3%	4%	0.10	0.01	112%	5%	23%
1,2,3-trichloropropane	0.35	0.11	103%	10%	5%	120%	19%	27%	0.49	0.13	98%	11%	4%	0.19	0.01	158%	2%	58%
n-propylbenzene	0.36	0.10	113%	17%	10%	138%	23%	20%	0.68	0.18	125%	16%	8%	0.10	0.01	112%	4%	25%
trans-1,4-dichloro-2-butene	0.14	0.11	0%	0%	0%	31%	24%	20%	0.20	0.16	0%	0%	0%	0.04	0.01	13%	2%	11%
1,3,5-trimethylbenzene	0.31	0.08	115%	9%	4%	123%	15%	17%	0.60	0.14	113%	10%	3%	0.09	0.01	97%	3%	20%
bromobenzene-d_5	0.29	0.08	94%	3%	5%	107%	6%	16%	0.52	0.14	97%	3%	4%	0.11	0.01	113%	4%	24%
bromobenzene	0.29	0.08	96%	3%	5%	108%	6%	16%	0.52	0.13	97%	3%	4%	0.11	0.00	113%	3%	24%
2-chlorotoluene	0.30	0.07	105%	3%	3%	115%	8%	16%	0.58	0.14	107%	4%	2%	0.09	0.01	98%	3%	21%
4-chlorotoluene	0.28	0.08	101%	4%	3%	110%	9%	15%	0.56	0.14	104%	5%	3%	0.09	0.01	98%	3%	20%
pentachloroethane	0.11	0.06	27%	54%	1%	45%	27%	8%	1.15	0.81	135%	75%	5%	0.01	0.01	13%	8%	3%
tert-butulbenzene	0.33	0.09	118%	19%	10%	134%	26%	19%	0.66	0.17	125%	19%	8%	0.09	0.01	104%	3%	22%
1,2,4-trimethylbenzene	0.29	0.07	112%	9%	5%	118%	15%	16%	0.56	0.13	107%	10%	4%	0.09	0.01	103%	2%	21%
sec-butylbenzene	0.33	0.09	114%	24%	15%	136%	28%	19%	0.69	0.17	133%	22%	13%	0.09	0.01	102%	3%	21%
aniline	0.87	0.32	80%	35%	37%	43%	17%	42%	0.53	0.20	57%	38%	15%	0.28	0.08	38%	13%	37%
p-isopropyltoluene	0.31	0.07	124%	21%	15%	134%	26%	20%	0.63	0.14	126%	20%	12%	0.08	0.01	106%	4%	24%
1,3-dichlorobenzene	0.24	0.05	94%	5%	7%	98%	3%	13%	0.50	0.11	98%	4%	5%	0.07	0.00	90%	2%	20%
1,4-dichorobenzene	0.23	0.05	93%	6%	7%	96%	3%	13%	0.49	0.11	96%	5%	6%	0.07	0.01	91%	2%	20%
n-butylbenzene	0.29	0.06	109%	22%	17%	124%	23%	18%	0.63	0.13	128%	20%	15%	0.08	0.01	96%	3%	22%
1,2-dichlorobenzene-d_4	0.21	0.05	90%	9%	10%	89%	5%	12%	0.47	0.11	95%	8%	8%	0.06	0.00	82%	1%	19%
1,2-dichlorobenzene	0.22	0.05	91%	10%	10%	90%	7%	12%	0.47	0.11	96%	9%	7%	0.07	0.00	85%	1%	19%
decafluorobiphenyl	0.20	0.05	97%	12%	14%	100%	26%	22%	0.48	0.09	100%	11%	13%	0.06	0.01	95%	10%	34%
n-nitrosodi-*n*-propylamine	0.99	0.16	288%	51%	47%	133%	61%	129%	0.83	0.15	179%	50%	21%	0.39	0.03	65%	5%	65%
nitrobenzene-d_5	0.40	0.13	374%	105%	283%	128%	23%	65%	0.57	0.14	176%	58%	40%	0.14	0.01	80%	5%	58%
acetophenone-d_5	0.63	0.16	216%	47%	28%	169%	34%	99%	0.77	0.18	187%	47%	19%	0.20	0.01	84%	5%	67%

o-toluidine	0.79	0.27	67%	39%	34%	62%	21%	56%	0.58	0.20	58%	41%	18%	0.22	0.05	53%	15%	48%
1,2-dibromo-3-chloropropane	0.27	0.13	97%	39%	12%	119%	46%	32%	0.55	0.20	107%	40%	10%	0.07	0.00	87%	4%	35%
hexachlorobutadiene	0.20	0.06	108%	27%	20%	104%	26%	25%	0.58	0.15	122%	28%	18%	0.04	0.00	60%	2%	25%
1,2,4-trichlorobenzene-d_3	0.16	0.04	89%	14%	13%	80%	11%	20%	0.43	0.11	92%	11%	10%	0.04	0.01	66%	4%	30%
1,2,4-trichlorobenzene	0.16	0.04	94%	12%	14%	81%	12%	19%	0.44	0.11	94%	9%	11%	0.04	0.00	67%	3%	28%
naphthalene-d_8	0.14	0.04	85%	14%	18%	80%	7%	31%	0.40	0.10	93%	12%	14%	0.05	0.00	84%	1%	52%
naphthalene	0.15	0.04	95%	11%	22%	76%	7%	19%	0.41	0.10	95%	9%	16%	0.05	0.00	76%	1%	33%
1,2,3-trichlorobenzene	0.14	0.04	88%	7%	22%	73%	12%	21%	0.43	0.12	96%	9%	18%	0.03	0.00	57%	3%	30%
n-nitrosodibutylamine	0.40	0.21	25%	99%	19%	65%	47%	47%	0.55	0.30	25%	115%	12%	0.12	0.02	76%	18%	56%
2-methylnaphthalene	0.19	0.05	194%	21%	74%	150%	18%	114%	0.43	0.11	96%	23%	26%	0.05	0.01	147%	17%	154%
1-methylnaphthalene-d_{10}	0.12	0.04	111%	13%	33%	182%	30%	193%	0.37	0.11	84%	11%	21%	0.04	0.01	190%	1%	208%

[a]One g samples were sonication spike with an overnight equilibration period (>1000 min) and 10 g samples were vacuum spiked with an overnight equilibration period (>1000 min) prior to analyses. The concentration of analytes in the 10 g samples are listed in Table 1. The concentration of analytes in the 1 g samples were 10 times the values listed in Table 1.
[b]Reference standards were prepared using 5 mL water as the matrix.
[c]Reference standards were prepared using 1 g tuna and 5 mL water as the matrix.
[d]Relative response ratio is the response of analytes from the sample divided by the analyte response from the standard. The deviation is 1 sigma.
[e]Recovery is the measured analyte relative response divided by the predicted surrogate-corrected relative response. The diviation is 1 sigma.
[f]Average predicted surrogate-correction precision.