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Stephen L R Ellison, Michael H Ramsey, Paul Lawrence, Brian Stuart, Jesus Minguez, Michael J Walker

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Is measurement uncertainty from sampling related to analyte concentration?

Electronic Supplementary Information

Stephen L R Ellison^a, Michael H Ramsey^b, Paul Lawrance^a, Brian Stuart^a, Jesus Minguez^a, and Michael J Walker^a

^a LGC limited, Queens Road, Teddington Middlesex TW11 0LY

^b School of Life Sciences, University of Sussex, Falmer, Brighton, UK, BN1 9QG

Tables 2 and 3 follow. References to sources for data in Table 3 are included after the two Tables.

Table 2: Literature study - Foodstuffs and methodology

Product	Analyte	Sampling	Sampling	Sampling	UfS Method -	Sample	Source
		Env/form	Target	Protocol	How dups	amount	
Dista abia muta	Tatal effeterin	Detail (sin als)	Detals of muta in	Trading Stda	taken	250 -	1
Pistachio nuts	1 otal allatoxin	ketall (single)	1 retailer over 4	Trading Stas	Duplicate: S1s	250 g	1
		loose in shells	deve	Officers	day 4		
Wheat	N	Wholesale	$1 \times 800 \text{ tons in}$	own	CTS(n-5) using	3000 g	2
wheat	Molybdenum (Mo)		hean	own	within-sampler	5000 5	2
	Lead (Ph)		neup		variance		
Coffee(Green)	Moisture	Wholesale	1 x 11 tons in	own	CTS (n=8) using	500 g	_
	Nickel (Ni)		185 sacks		within-sampler		
	Yttrium (Y)				variance		
Milk	(Added) Water	Retail (multiple)	Batches in 9	Trading Stds	Duplicate (n=9),	568 or 500	3
			retailers over 4	Officer's	2 visits	ml	
			days				
Spreadable fats	Fat	Retail (multiple)	Batches in 9	Trading Stds	Duplicate (n=8),	250-500g	3
			retailers over 4	Officer's	2 visits		
			days				
Sausages	Meat	Retail (multiple)	Batches in 9	Trading Stds	Duplicate (n=9),	500 g	3
	Fat		retailers over 4	Officer's	2 visits		4 p260-1
	Moisture		days				4 p260-1
	Ash						4 p260-1
	N						4 p260-1
Apples	Propargite (pesticide)	Wholesale	230kg in 14	Modified Dpt. of	Duplicate (n=9	2 kg	4 p102
			boxes from 14	Health	boxes)		
			wholesalers				
Strawberries	Pyrimethanil	Retail (multiple)	Fruit avaiable	Modified CSL	Duplicate (n=9	2 kg	5
	Chlorothalonil		for retail from	(pesticide R&D	boxes)		
	Tolyfluanid		shops and street	team)			
	Myclobutanil		market stalls				
	Bupirimate						
	Kresoxim-methyl						
	Fenhexamid						

 Table 2 (Continued)

Product	Analyte	Sampling Env/form	Sampling Target	Sampling Protocol	UfS Method - How dups taken	Sample amount	Source
Infant milk	Zinc (Zn) Lead (Pb) Copper (Cu) Cadmium (Cd)	Retail (multiple)	Those avaiable for retail from shops in York area	Modified MAFF(later DEFRA) survey	Duplicate (n=10 containers)	Single pots (mass unknown)	6
	Arsenic(As) Tin(Sn)	_					4 p265
Infant wet meals	Zinc (Zn) Lead (Pb) Copper (Cu) Cadmium (Cd)	Retail (multiple)	Those avaiable for retail from shops inYork area	Modified MAFF(later DEFRA) survey	Duplicate (n=10 containers)	Single pots (mass unknown)	6
Butter(frozen)	Fat Fat Solids-not-fat (SNF) Solids-not-fat (SNF) Free fatty acids (FFA) Free fatty acids (FFA) Moisture Peroxide value (PV » rancidity). Peroxide value (PV » rancidity).	Wholesale	20 tons (800x25kg blocks)	Modified EC 2571/97 + 2771/1999 Annex IV	Duplicate (n=8) balanced design	112 g _3 cores 1575 g 112g_3 cores g 1575 g ~112 g - 3 cores ~112 g - 3 cores ~112 g - 3 cores ~112 g - 3 cores ~1575 g - 3 cores ~1575 g - 3 cores ~112 g _3 cores ~12 g _3 cores ~172 g _3 cores	7, 8

Table 2 (Continued)

Product	Analyte	Sampling	Sampling	Sampling	UfS Method -	Sample	Source
		Env/form	Target	Protocol	How dups taken	amount	
Lettuce (glasshouse,	Nitrate	Grower	8 batches of	EC/2002/63	Duplicate (n=8)	10 heads	9, 10 p86
ex. Iceberg)		(glasshouse)	2000 - 12,000		balanced design	(Nov)	-
			growing plants			10 heads	
						(Feb/Mar)	-
			A 1111 1	EC/2001/22	\mathbf{D} \mathbf{I} (0)	40 head	10
Tuna (fresh)	Mercury (Hg)	Retail (multiple)	Available in	EC/2001/22	Duplicate (n=8)	~350 g	10
Tuna (tinned)	Mercury (Hg)	Retail (multiple)	retail outlets in		balanced design	~350 g (2	10 p134
	Managamy (IIa)	Datail (multipla)	one area			$\frac{\text{uns}}{1200} \approx (8)$	10 = 124
	Mercury (Hg)	Retail (multiple)				$1200 g(\delta$	10 p154
Tomatoes (tinned)	Tin (Sn)	Retail (multiple)	Available in	EC/2004/16	Duplicate $(n-8)$	500 g (P1)	10 p124
Tomatoes (timed)	Tin (Sn)	Retail (multiple)	retail outlets in	LC/2004/10	balanced design	500 g (R1)	10 p124
	Tin (Sn)	Retail (multiple?)	one area		ouruneed design	4000 g	10 P137
Laver meal feed	Calcium (Ca)	Factory	1 lot of ~100	Manufacturer's	Duplicate (n=8)	~200 g	10 P149.
,	Sodium (Na)		tons, made up of		balanced design	8	p156, p170,
	Salt (NaCl)		n loads		8		p182
	Copper (Cu)						-
Chicken feed	Enzyme	Wholesale	25 kg bag	own	Modelling using	500g (2g	11 p71
					Gy eqn.	sub-sample)	
Apple Juice (cloudy)	Patulin	Factory	1 x 6,500 litres	Manufacturers	SPT (n=9)	220 ml	12
Butter (fresh)	Moisture	Factory	1 x 20.1 tons	RPA	SPT (n=9)	6 x100g	12
Com (shallad)	Aflataria	Wholesele	10 lota		Empirical	1 12 1-2 (50	12
Corn (snelled)	Anatoxin	wholesale	18 1018	OWI	Empiricai	sub-sample)	15
	Aflatoxin	Wholesale	?	own	Empirical	0.91 kg	14
	Aflatoxin	Wholesale	?	own	Empirical	0.91 kg	15
Peanut	Aflatoxin	Wholesale	?	own	Empirical	5 kg	16
		Wholesale	40 lots of 900 kg	own	Empirical	2.27kg (sub- sample 100g)	17

 Table 2 (Continued)

Product	Analyte	Sampling Env/form	Sampling Target	Sampling Protocol	UfS Method - How dups	Sample amount	Source
					taken		
Coffee (green)	Ochratoxin A	Wholesale	25 lots of unkown mass	own	Empirical unbalanced (25 x 16 x 1or2 x 1or2)	16kg	18
Wheat	Deoxynivalenol(DON)	Wholesale		own	Empirical	0.454 kg (25g sub- sample)	19
Hazelnuts	Aflatoxin (total)	Wholesale	20 lots (of unkown mass)	own	Empirical	10kg (x 16)	20

Note 1: CTS rather than duplicate method used. If significant between-sampler contribution added, s_{samp} increase to 0.0418 (for N) and 0.0613 (for Mo), increasing U_{meas}% to 3.95 (for N) and 26.3 for (Mo) (calc by

Ramsey, 2009)

Table 3: Literature study - sampling uncertainties

Product	Analyte	Units	Sample	S produc	s samp	s samp	s anal	s meas	mean	$s_{samp}^2 + s_{prep}^2$	U _{meas} %	U _{samp} %	U _{anal} %	Source
			amount	t		hich			conc	s_{meas}^2				
Pistachio	Total aflatoxin	ug kg-1	250 g	0.228	0.194	include	0.233	0.303	0.86	0.41	70.45	45.02	54.19	1
nuts						d in								
						Ssamp								
Wheat	N	% m/m	3000 g		0.022	"	0.005	0.02	2.13	0.95	2.08	2.03	0.47	2
	Molybdenum (Mo)	mg kg ⁻¹			0.029	"	0.015	0.03	0.48	0.79	13.60	12.08	6.25	
	Lead (Pb)	mg kg ⁻¹			0.007	"	0.005	0.01	0.017	0.67	93.68	76.47	54.12	
Coffee(G	Moisture	% m/m	500 g		0.099	"	0.109	0.15	11.98	0.45	2.46	1.65	1.82	
reen)	Nickel (Ni)	mg kg ⁻¹			0.540	"	0.530	0.76	4.83	0.51	31.33	22.36	21.95	
	Yttrium (Y)	mg kg ⁻¹			0.006	"	0.000	0.01	0.0124	0.99	90.61	90.32	7.26	
Milk	(Added) Water	(m°C)	568 or		2.290	"	0.690	2.392	543.79	0.92	0.88	0.84	0.25	3
			500 ml											
Spreadab	Fat	% m/m	250-		0.490	"	0.400	0.633	57.78	0.60	1.09	1.70	1.38	3
le fats			500g											
Sausages	Meat	% m/m	500 g		3.470	"	1.150	3.656	69.17	0.90	11.28	10.03	3.33	3
	Fat	% m/m		5.027	1.382	"	0.434	1.45	21.36	0.91	13.56	12.94	4.06	4 p260-1
	Moisture	% m/m		5.347	1.419	"	0.377	1.47	55.89	0.93	5.25	5.08	1.35	4 p260-1
	Ash	% m/m		0.3205	0.032	"	0.000	0.03	2.5	1.00	2.59			4 p260-1
	Ν	% m/m		0.2956	0.039	"	0.034	0.05	1.862	0.57	5.58			4 p260-1
Apples	Propargite	mg kg ⁻¹	2 kg	0.2857	0.091	"	0.126	0.155	0.6746	0.34	46	26.98	37.36	4 p102
	(pesticide)		_											_
Strawber	Pyrimethanil	mg kg ⁻¹	2 kg		0.0481	0.0316	0.028	0.064	0.2243	0.81	57.07	42.89	24.97	5
ries	Chlorothalonil	mg kg ⁻¹			0.0005	0	0.0005	0.001	0.001	0.25	200.00	100.00	100.00	
	Tolyfluanid	mg kg ⁻¹			0.0025	0.0026	0.0021	0.004	0.0124	0.81	64.52	40.32	33.87	
	Myclobutanil	mg kg ⁻¹	1		0.0063	0.0077	0.0045	0.011	0.0305	0.82	72.13	41.31	29.51	1
	Bupirimate	mg kg ⁻¹	1		0.0134	0.0237	0.0089	0.029	0.0713	0.88	81.26	37.55	25.11	1
							6		8					
	Kresoxim-methyl	mg kg ⁻¹	1		0.0008	0.0003	0.0012	0.0014	0.0017	0.37	164.71	94.12	141.18	1
	Fenhexamid	mg kg ⁻¹	1		0.0486	0.0084	0.0326	0.059	0.2257	0.70	52.28	43.07	28.89	1

Table 3 (Continued)

Product	Analyte	Units	Sample amount	s produc t	s samp	s samp prep*	s anal	s meas	mean conc	$\frac{s_{samp}^2 + s_{prep}^2}{s_{meas}^2}$	U _{meas} %	U _{samp} %	U _{anal} %	Source
Infant milk	Zinc (Zn)	ug kg ⁻¹	Single pots (mass	12810	0	include d in s samp	4346	4346	49931	0.00	17.4	0.00	17.41	6
	Lead (Pb)	ug kg ⁻¹	unkown)	0.5815	0	"	1.271	1.271	4.815	0.00	52.8	0.00	52.79	
	Copper (Cu)	ug kg ⁻¹		581.6	63.38	"	184.8	195.4	2806	0.11	13.9	4.52	13.17	
	Cadmium (Cd)	ug kg ⁻¹		5.241	0.244	"	1.006	1.035	4.654	0.06	44.5	10.49	43.23	
	Arsenic(As)	ug kg ⁻¹		5.936	2.341	"	2.28	3.27	10.29	0.51	63.51	45.50	44.31	4 p265
	Tin(Sn)	ug kg ⁻¹		408.43	189.22	"	43.57	194.17	358.8	0.95	108.23	105.47	24.29	
Infant	Zinc (Zn)	ug kg ⁻¹	Single		431.5	"	506.1	665.1	4019.5	0.42	33.1	21.47	25.18	6
wet	Lead (Pb)	ug kg ⁻¹	pots		1.322	"	2.275	2.631	4.884	0.25	107.7	54.14	93.16	
meals	Copper (Cu)	ug kg ⁻¹	(mass		77.92	"	30.19	83.57	493	0.87	33.9	31.61	12.25	
	Cadmium (Cd)	ug kg ⁻¹	unkown)		1.235	"	1.1	1.654	7.575	0.56	43.7	32.61	29.04	
Butter (frozen)	Fat	% m/m	112 g _3 cores	0.252	0.2165	"	0.0568	0.2238	82.92	0.94	0.54	0.52	0.14	7, 8
, ,	Fat	% m/m	1575 g	0.374	0.151	"	0.046	0.158	83.19	0.91	0.54	0.36	0.11	
	Solids-not-fat (SNF)	% m/m	112g_3 cores g	0.035	0.0495	"	0.0399	0.0636	1.34	0.61	9.48	7.39	5.96	
	Solids-not-fat (SNF)	% m/m	1575 g	0.138	0.08	"	0.041	0.09	1.28	0.79	9.48	12.50	6.41	
	Free fatty acids (FFA)	% m/m	~112 g - 3 cores	0.031	0.0035	"	0.0057	0.0067	0.295	0.27	4.51	2.37	3.86	
	Free fatty acids (FFA)	% m/m	~672 g - 3 cores	0.009	0.001	"	0.001	0.01	0.28	0.01	4.51	0.71	0.71	
	Moisture	% m/m	~112 g - 3 cores	0.25	0.1947	"	0.0421	0.1992	15.755	0.96	2.53	2.47	0.53	
	Moisture	% m/m	~1575 g - 3 cores	0.379	0.1550	"	0.0360	0.0159	15.556	95.03	2.53	1.99	0.46	
	Peroxide value (PV » rancidity).	meq. kg ⁻¹	~112 g _3 cores	0	0.024	"	0.0108	0.0263	0.083	0.83	63.3	57.83	26.02	
	Peroxide value (PV » rancidity).	meq. kg ⁻¹	~672 g _3 cores	0	0.044	"	0.007	0.044	0.084	1.00	63.3	104.76	16.67	

Table 3 (Continued)

Product	Analyte	Units	Sample amount	s produc	s samp	s samp prep*	s anal	s meas	mean conc	$\underline{s_{samp}^2 + s_{prep}^2}$	U _{meas} %	U _{samp} %	U _{anal} %	Source
				t		I I				s_{meas}^2				
Lettuce	Nitrate	mg kg ⁻¹	10 heads	565.4	319.05	"	167.9	360.55	4408	0.78	16.4	14.48	7.62	9, 10
glasshouse			(Nov)					1						p86
ex.			10 heads	580.2	553.51	"	53.85	556.13	3148.3	0.99	35.3	35.16	3.42	
Iceberg			(Feb/Ma											
			r)	10.1.2						0.00	10.0	10.11		
		1	40 head	694.3	306.16		42.2	309.06	3117.5	0.98	19.8	19.64	2.71	1.0
Tuna	Mercury (Hg)	mg kg ⁻¹	~350 g	0.07	0.027	"	0.008	0.028	0.257	0.93	21.79	21.01	6.23	10
(fresh)		1 -1	250	0.1.40	0.015		0.007	0.017	0.000	0.70	1675	1470	5.01	10 124
Tuna (time al)	Mercury (Hg)	mg kg ⁻¹	$\sim 350 \text{ g}$	0.142	0.015		0.006	0.017	0.203	0.78	16.75	14.78	5.91	10 p134
(tinned)	Manayary (IIa)	ma 1.a-1	(2 tins)	0.202	0.015	"	0.002	0.016	0.222	0.88	12 72	12.00	2.59	10 = 124
	Mercury (Hg)	ing kg -	1200 g (8 tins)	0.205	0.015		0.005	0.010	0.255	0.88	15.75	12.00	2.38	10 p154
Tomatoe	Tin (Sn)	ma ka-1	500 σ	1 987	2 4 2 6	"	0.829	2 564	6.455	0.90	79 44	75 17	25.69	10 n124
s (tinned)		III5 K5	(R1)	1.907	2.420		0.027	2.304	0.435	0.90	17.77	13.17	23.07	10 p124
s (tillieu)	Tin (Sn)	mg kg ⁻¹	500 g	21.19	7.3	"	2.23	7.63	74.26	0.92	20.55	19.66	6.01	10 p137
			(R2)		110			1100	/0	0.72	-0.00	17100	0.01	10 110 /
	Tin (Sn)	mg kg ⁻¹	4000 g	23.95	15.61	"	2.34	15.78	78.09	0.98	40.41	39.98	5.99	10 P137
Layer	Calcium (Ca)	mg kg ⁻¹	~200 g	8072	5807	"	528.4	5831	42169	0.99	27.66	27.54	2.51	10 P149,
meal feed	Sodium (Na)	mg kg ⁻¹		179.8	226.5	"	30.43	228.55	1676	0.98	27.27	27.03	3.63	156,
	Salt (NaCl)	% m/m		0	0.081	"	0.021	0.084	0.353	0.93	47.59	45.89	11.90	170, 182
	Copper (Cu)	mg kg ⁻¹		2.27	0.96	"	1.31	1.63	14.93	0.35	21.84	12.86	17.55	
Chicken	Enzyme	% m/m	500g (2g		0.0016	0.0065	0.0025	0.01	0.05	0.88	28.63	6.60	10.00	11 p71
feed			sub-		5									
			sample)											
Apple	Patulin	ug l ⁻¹	220 ml	n.a.	0 (n.d.)	"	5.1	5.1	52.6	0.00	19.4	0(n.d.)	19.39	12
Juice														
(cloudy)														
Butter	Moisture	% m/m	6 x100g	n.a.	0.052	"	0.03	0.06	15.41	0.75	0.78	0.67	0.39	12
(fresh)					0.08	"	0.03	0.086	15.41	0.87	1.12	1.04	0.39	

Table 3 (Continued)

Product	Analyte	Units	Sample	S	s samp	s samp	s anal	s meas	mean	$s_{samp}^2 + s_{prep}^2$	Umeas	Usamp	Uanal	Source
			amount	produc		prep*			conc	$\frac{sump}{s_{maas}^2}$	%	%	%	
				t						meus				
Corn	Aflatoxin	ug kg ⁻¹	1.13 kg		14.63	7.5	2.14	16.58	20	0.98	165.79	146.30	21.40	13
(shelled)			(50g sub-											
			sample)											
	Aflatoxin	ug kg-1	0.91 kg		16.4	7.5	5.5	18.85	20	0.91	188.54	164.00	55.00	14
	Aflatoxin	ug kg-1	0.91 kg		11.1	4.83	1.45	12.19	10	0.99	243.84	222.00	29.00	15
					328.2	388.3	79	514.52	10000	0.98	10.29	6.56	1.58	-
Peanut	Aflatoxin	ug kg ⁻¹	5 kg		22.8	7.69	7.08	25.08	20	0.92	250.82	228.00	70.80	16
					11.4	5.08	4.48	13.26	20	0.89	132.60	114.00	44.80	-
			2.27kg		153.4	42.8	3.87	159.31	100	1.00	318.61	306.80	7.74	17
			(sub-											
			sample											
			100g)											
Coffee	Ochratoxin A	ug kg ⁻¹	16kg		2.79	1.685	0.332	3.28	5	0.99	131.05	111.60	13.28	18
(green)														
Wheat	Deoxynivalenol	ppm (?)	0.454 kg		0.315	0.5	0.265	0.65	5	0.83	25.906	12.60	10.60	19
	(DON)		(25g											
			sub-											
			sample)											
Hazelnuts	Aflatoxin (total)	ug kg ⁻¹	10kg (x		13.19	0.86	0.52	13.23	10	1.00	264.56	263.80	10.40	20
			16)								5			

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