

1 **Table S1 – Comparison of the accuracy of ICP-MS, DMA-80 and pXRF analysis. ICP-MS: As, Cr,**  
 2 **Cu, Fe, Mn, Pb, Sb, Zn; DMA-80: Hg.**

CRM		As	Cr	Cu	Fe	Hg	Mn	Pb	Sb	Zn
PACS-3	CRM concentration (mg/kg)	30.3	90.6	356	41060	2.98	432	188	14.7	376
	pXRF average recovery (%)	164%	120%	104%	107%		107%	93%		109%
	Confirmatory analysis average recovery (%)	98%	96%	83%	95%	102%	93%	95%	99%	96%
MESS-4	CRM concentration (mg/kg)	21.7	94.3	32.9	37900	0.09	298	21.5	1.07	147
	pXRF average recovery (%)	121%	106%	160%	102%		103%	93%		102%
	Confirmatory analysis average recovery (%)	91%	98%	87%	89%	96%	91%	101%	85%	94%

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5 **Table S2 - Linear regression and t-test carried out on log<sub>10</sub> transformed data.**

Matrix type	Element	Preparation	Data quality <sup>a</sup>	n	RSD%	r <sup>2</sup>	T-test	Slope z-test		Y-int z-test	
								p-value			
Cu-Sb	As	Lab-prepared	Quantitative	37	7%	0.963*	0.000	0.527	0.185		
		Fast lab-prepared	Quantitative	37	7%	0.917*	0.000	0.485	0.149		
	Cr	Lab-prepared	Qualitative	25	12%	0.523*	0.021	0.721	0.720		
		Fast lab-prepared	Qualitative	21	14%	0.249	0.282	0.610	0.531		
	Cu	Lab-prepared	Quantitative	37	8%	0.979*	0.000	0.641	0.201		
		Fast lab-prepared	Quantitative	37	5%	0.963*	0.000	0.650	0.104		
	Fe	Lab-prepared	Quantitative	37	1%	0.970*	0.000	0.731	0.410		
		Fast lab-prepared	Quantitative	37	1%	0.933*	0.000	0.079	0.000		
	Hg	Lab-prepared	Quantitative	11	14%	0.959*	0.127	0.802	0.637		
		Fast lab-prepared	Quantitative	13	11%	0.885*	0.207	0.539	0.367		
	Mn	Lab-prepared	Quantitative	37	3%	0.929*	0.004	0.605	0.458		
		Fast lab-prepared	Quantitative	37	4%	0.875*	0.002	0.554	0.403		
	Pb	Lab-prepared	Definitive	37	6%	0.988*	0.760	0.770	0.524		
		Fast lab-prepared	Definitive	37	5%	0.919*	0.066	0.867	0.920		
	Sb	Lab-prepared	Definitive	15	9%	0.970*	0.576	0.704	0.589		
		Fast lab-prepared	Definitive	12	7%	0.940*	0.980	0.707	0.613		
	Zn	Lab-prepared	Quantitative	37	4%	0.969*	0.007	0.849	0.709		
		Fast lab-prepared	Quantitative	37	3%	0.933*	0.000	0.809	0.573		
Pb-Zn	As	Lab-prepared	Quantitative	52	10%	0.856*	0.000	0.383	0.051		
		Fast lab-prepared	Qualitative	52	12%	0.699*	0.001	0.371	0.096		
	Cr	Lab-prepared	Qualitative	5	7%	0.100	0.007	0.035	0.000		
		Fast lab-prepared	Qualitative	5	8%	0.079	0.024	0.100	0.007		
	Cu	Lab-prepared	Qualitative	34	16%	0.358*	0.000	0.024	0.001		
		Fast lab-prepared	Qualitative	43	17%	0.233	0.000	0.016	0.000		
	Fe	Lab-prepared	Quantitative	53	1%	0.952*	0.000	0.201	0.003		
		Fast lab-prepared	Quantitative	51	3%	0.874*	0.000	0.158	0.002		
	Hg	Lab-prepared	Qualitative	7	11%	0.050	0.000	0.537	0.017		
		Fast lab-prepared	Qualitative	6	9%	0.001	0.000	0.381	0.104		
	Mn	Lab-prepared	Quantitative	57	7%	0.895*	0.003	0.917	0.747		
		Fast lab-prepared	Quantitative	49	12%	0.806*	0.233	0.799	0.646		
	Pb	Lab-prepared	Definitive	58	5%	0.993*	0.370	0.789	0.718		
		Fast lab-prepared	Quantitative	55	5%	0.907*	0.013	0.620	0.622		
	Sb	Lab-prepared	Qualitative	2	n.d.	n.d.	n.d.	n.d.	n.d.		
		Fast lab-prepared	Qualitative	2	n.d.	n.d.	n.d.	n.d.	n.d.		
	Zn	Lab-prepared	Definitive	58	4%	0.992*	0.053	0.887	0.711		
		Fast lab-prepared	Definitive	56	5%	0.910*	0.508	0.591	0.422		

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7 <sup>a</sup> Data quality levels are defined by US EPA [10]

8 \* Significant for p < 0.001

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