

Multi-energy calibration and aerosol dilution as analytical strategies to access the in vitro bioaccessibility of essential elements and arsenic in raw and cooked shrimp by plasma-based methods

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Supplementary Material

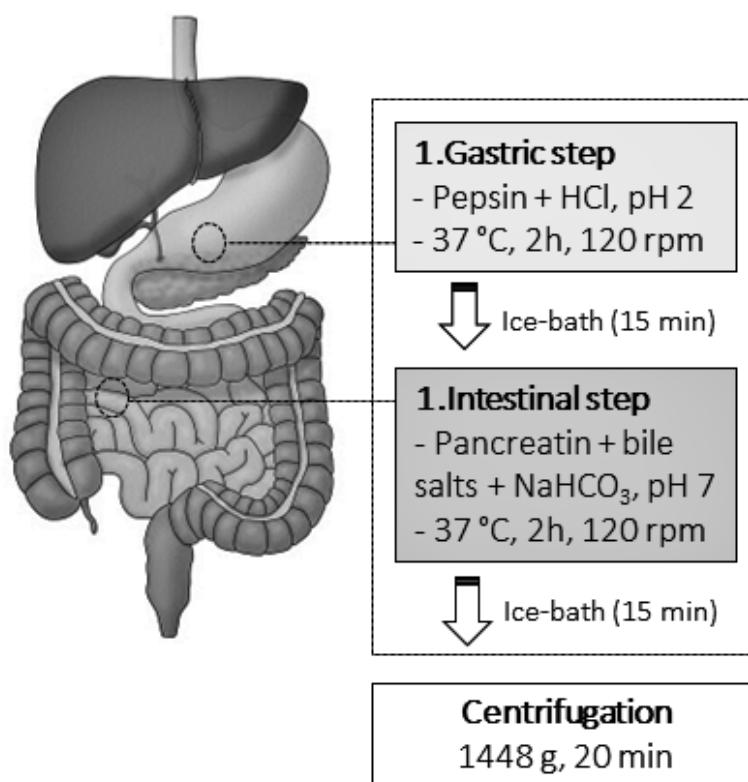


Figure S1. Schematic representation of the in vitro digestion model

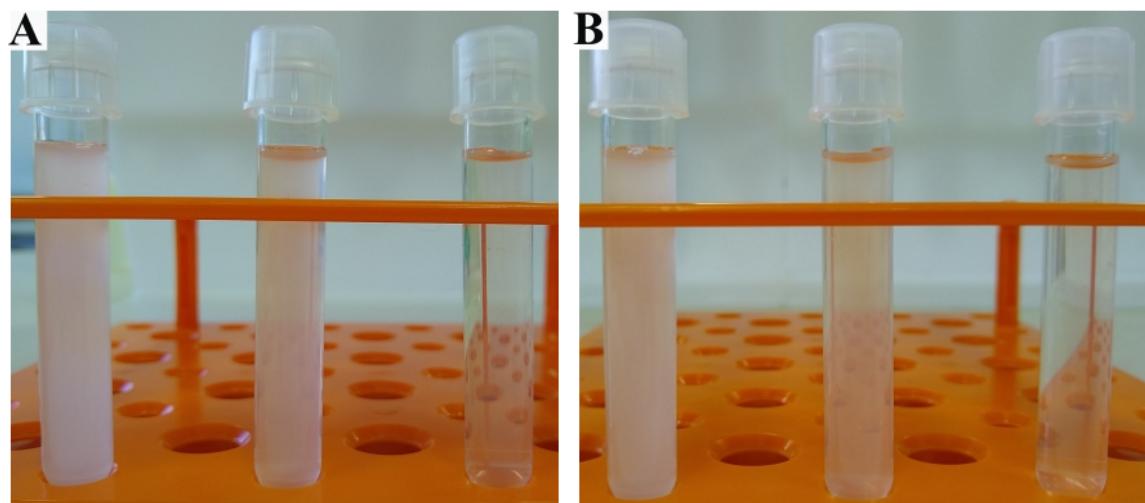


Figure S2. Physical aspect of the chyme after dilution in 1 % v v¹ HNO₃. (A) raw sample. (B) cooked sample. Dilution factors at 1:2.5, 1:5, and 1:10 are shown from left to right.

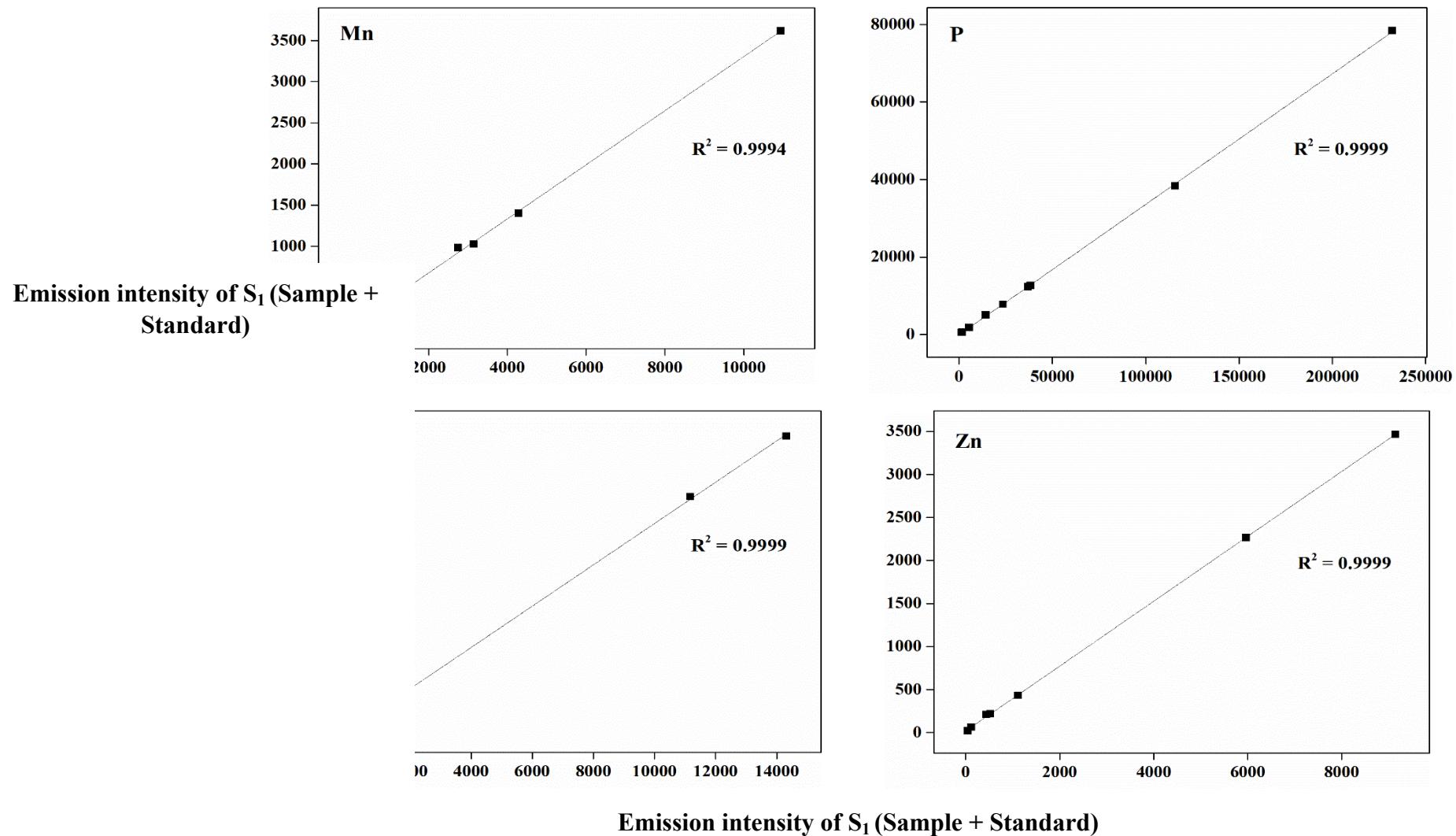


Figure S3. Calibration plots obtained from MEC-ICP OES for Mn, P, S, and Zn. Each x-y pair refers to a calibration point obtained by running S_1 and S_2 at the optimized conditions.

Table S1. Analytical figures of merit of the procedure for total mass fraction determination by ICP OES

Analyte				Trueness					
	LOD (mg kg ⁻¹ ww)	LOQ (mg kg ⁻¹ ww)	Precision (% RSD)	CRM TORT-3			CRM DOLT-5		
				Found value (mg kg ⁻¹)	Certified value (mg kg ⁻¹)	t _{calc.} *	Found value (mg kg ⁻¹)	Certified value (mg kg ⁻¹)	t _{calc.} *
Ca	9 – 13	28 – 41	1.1	2415 ± 27	nc	-	577 ± 14	550 ± 80	3.43
Cu	0.1	0.3 – 0.4	1.1	478 ± 17	497 ± 22	2.03	35.3 ± 0.6	35.0 ± 2.4	0.98
Fe	0.1	0.2 – 0.3	3.5	163 ± 7	179 ± 8	3.76	1114 ± 30	1070 ± 80	2.55
Mg	17 – 24	50 – 72	0.7	1105 ± 10	nc	-	924 ± 22	940 ± 100	1.28
Mn	0.1	0.2	2.0	14.3 ± 0.7	15.6 ± 1.0	3.34	8.69 ± 0.20	8.91 ± 0.70**	1.91
P	201 – 287	610 – 871	1.0	10621 ± 72	nc	-	11991 ± 210	11500***	4.06
S	78 – 112	237 – 338	0.8	15886 ± 245	nc	-	20688 ± 325	nc	-
Zn	0.4 – 0.5	1.1 – 1.5	0.9	130 ± 3	136 ± 6	3.05	106.3 ± 2.6	105.3 ± 5.4	0.65
As	0.1	0.2	1.8	63.3 ± 4.8	59.5 ± 3.8	2.76	32.3 ± 1.0	34.6 ± 2.4	3.20

*t_{calc.} = calculated t-value at a 95 % of confidence level (t-critical = 4.30). nc = no certified. ** reference value. *** information value.

Table S2: Total dissolved solids in the chyme after *in vitro* digestion

Component	Concentration (% m/v)	Final concentration in the chyme (% m/v)
Pepsin	10	0.16
Pancreatin	0.2	0.04
Bile salts	1.3	0.24
NaHCO ₃	0.8	0.16
NaOH	4.0	0.16
Sample	-	2.0*

$$\text{TDS (%m/v)} = 2.8$$

* Assuming a sample dissolution of about 50 %.

Table S3. Mass balance study for raw and cooked shrimp.

Element	Raw shrimp (mg kg ⁻¹ dry-weight)				Cooked shrimp (mg kg ⁻¹ dry-weight)			
	Total mass fraction	Bioaccessible fraction	Residual fraction	MB (%)	Total mass fraction	Bioaccessible fraction	Residual fraction	MB (%)
Ca	4,094 ± 24	3,082 ± 137	687 ± 62	92	2,902 ± 43	2,291 ± 53	734 ± 26	104
Cu	6.0 ± 0.1	3.2 ± 0.1	2.7 ± 0.2	98	4.3 ± 0.1	3.2 ± 0.2	1.2 ± 0.1	104
Fe	39.4 ± 0.5	7.8 ± 0.2	23.5 ± 0.8	80	24.7 ± 0.3	6.7 ± 0.2	14.1 ± 0.9	84
Mg	2,026 ± 20	1,559 ± 46	262 ± 19	90	1,251 ± 18	976 ± 11	161 ± 5	91
Mn	4.7 ± 0.1	3.0 ± 0.1	1.3 ± 0.1	92	2.7 ± 0.1	1.7 ± 0.1	0.95 ± 0.08	98
P	9,642 ± 135	7,502 ± 225	1,562 ± 103	94	6,062 ± 50	4,619 ± 72	834 ± 31	90
S	12,723 ± 146	8,312 ± 286	3,089 ± 154	90	8,384 ± 58	4,967 ± 40	2,771 ± 38	92
Zn	56.3 ± 0.3	15.0 ± 0.2	40.0 ± 2.7	98	39.8 ± 0.2	5.9 ± 0.7	31.0 ± 0.6	93
As	2.5 ± 0.1	1.9 ± 0.1	0.56 ± 0.03	97	1.7 ± 0.1	1.1 ± 0.1	0.35 ± 0.05	85

MB = mass balance