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Supplementary Information

Solubility and Bioaccessibility of Ba, Ca, Cr, Cu, Fe, Mg, Mn, P, Sr and Zn in Slim Coffee Infusions by *in vitro* Gastrointestinal Digestion

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Table S1. Conditions of the *in vitro* gastrointestinal digestion of different food samples

Sample	Analyte	Simulated gastric juice (SGJ)	Simulated intestinal juice (SIJ)	Experimental details	Detection	Reference
Hazelnut, walnut, kernels	Cd, Cu, Fe, Mn, Pb, Zn	1% (m/v) pepsin in 0.01 mol L^{-1} HCl (pH 2)	3% (m/v) pancreatin + 1% (m/v) amylase + 0.15% (m/v) bile salt in H_2O	sample: 5 g SGJ: 50 mL incubation (37 °C, 4 h, shaking) pH 7.4 ($NaHCO_3$) SIJ: 50 mL incubation (37 °C, 4 h, shaking) centrifugation filtration (45 mm)	FAAS	1
Human milk, infant formulas	Fe, Zn	0.02% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.015% (m/v) pancreatin in 0.1 mol L^{-1} $NaHCO_3$	sample: 20 mL (human milk), 30 mL (infant formulas) SGJ: 1 mL incubation (37 °C, 50 min, shaking) an ice-water bath - stopping the digestion sample: 15 mL gastric digest pH 7.0 (1.5 mol L^{-1} $NaHCO_3$) SIJ: 1 mL incubation (37 °C, 30 min, shaking) an ice-water bath - stopping the digestion centrifugation (15300 rpm, 30 min, 4 °C)	FAAS	2
First-age infant formulae, human milk	Ca, Fe, Zn	10% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.3% (m/v) pancreatin + 0.7% (m/v) bile salt in 0.1 mol L^{-1} $NaHCO_3$	sample: 100 g pH 4.0 (6 mol L^{-1} HCl) SGJ: 3 mL incubation (37 °C, 2 h, shaking) sample: 50 g suspension pH 5.0 (1 mol L^{-1} $NaHCO_3$) dialysis (37 °C, 30 min, shaking, 1 kDa) pH 7.5 (1 mol L^{-1} $NaHCO_3$) SIJ: 15 mL dialysis (37 °C, 2 h, shaking, 1 kDa)	FAAS, ETAAS	3

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Table S1. Conditions of the *in vitro* gastrointestinal digestion of different food samples (cont.)

Sample	Analyte	Simulated gastric juice (SGJ)	Simulated intestinal juice (SIJ)	Experimental details	Detection	Reference
School meals	Ca, Cu, Fe, Zn	16% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.4% (m/v) pancreatin + 2.5% (m/v) bile salt in 0.1 mol L^{-1} $NaHCO_3$	dialysis method: sample: 40 g + 60 g deionized H_2O pH 2.0 (6 mol L^{-1} HCl) SGJ: 5 g incubation (37 °C, 2 h, shaking) sample: 30 mL gastric digest + 25 mL H_2O + $NaHCO_3$ (pH 7.5) dialysis (37 °C, 45 min, shaking, 10-12 kDa) SIJ: 7.5 mL dialysis (37 °C, 75 min, shaking, 10-12 kDa) --- solubility method: sample: 30 g + 70 mL deionized H_2O pH 2.0 (6 mol L^{-1} HCl) SGJ: 5 g incubation (37 °C, 2 h, shaking) pH 5.0 (1 mol L^{-1} $NaHCO_3$) SIJ: 18.8 mL incubation (37 °C, 2 h, shaking) an ice-water bath - stopping the digestion pH 7.2 (0.5 mol L^{-1} NaOH) centrifugation (3500 g, 1 h, 4 °C)	FAAS, GFAAS	4
Blood orange juice	B, Cr, Cu, Fe, Mn, Mo, Se, Zn	12% (m/v) pepsin in H_2O	2% (m/v) pancreatin + 1% (m/v) bile salt	sample: 25 g SGJ: 50 g pH 1.7 (800 µL 6 mol L^{-1} HCl) H_2O (up to 100 mL) incubation (37 °C, 3 h, shaking) an ice-water bath - stopping the digestion centrifugation (12000 g, 2 h, 4 °C) ultrafiltration (4000 g, 4 °C, 3 kDa) --- sample: 50 g gastric digest pH 7.0 (10 mL NH_4HCO_3) SIJ: 40 g H_2O (up to 100 mL) incubation (37 °C, 4 h, shaking) an ice-water bath - stopping the digestion centrifugation (12000 g , 2 h, 4 °C) ultrafiltration (4000 g, 4 °C, 3 kDa)	ICP OES, GFAAS	5
Soybean milk	Ca	16% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.4% (m/v) pancreatin + 2.5% (m/v) bile salt in 0.1 mol L^{-1} $NaHCO_3$	sample: 200 mL pH 2.0 (6 mol L^{-1} HCl) SGJ: 3 mL incubation (37 °C, 2 h) --- sample: 20 mL gastric digest + 25 mL H_2O + $NaHCO_3$ (pH 7.5) dialysis (37 °C, 30 min, shaking, 10-12 kDa) SIJ: 5 mL dialysis (37 °C, 75 min, shaking, 10-12 kDa)	FAAS	6

Table S1. Conditions of the *in vitro* gastrointestinal digestion of different food samples (cont.)

Sample	Analyte	Simulated gastric juice (SGJ)	Simulated intestinal juice (SIJ)	Experimental details	Detection	Reference
Milk-based fruit beverages	Ca, P	0.02 g pepsin *per* g sample	(0.005 g pancreatin + 0.03 g bile salt) *per* g sample	solubility method: sample: 80 g pH 2.0 (6 mol L^{-1} HCl) SGJ: 0.02 g pepsin *per* g sample H_2O (up to 100 mL) incubation (37 °C, 2 h, shaking) an ice-water bath - stopping the digestion --- pH 7.4 ($NaHCO_3$) SIJ: 0.005 g pancreatin + 0.03 g bile salt *per* g sample incubation (37 °C, 2 h, shaking) an ice-water bath - stopping the digestion pH 7.2 (0.5 mol L^{-1} NaOH) heating (100 °C, 4 min) centrifugation (3500 g, 1 h, 4 °C)	FAAS	7
Whole cashew apple juice, cashew apple fiber	Cu, Fe, Zn	16% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.4% (m/v) pancreatin + 2.5% bile salt in 0.1 mol L^{-1} $NaHCO_3$	sample: 20 g + 100 mL 0.01 mol L^{-1} HCl pH 2 (2 mol L^{-1} HCl) SGJ: 3.2 mL incubation (37 °C, 1 h, shaking) --- pH 7.5 (NaOH) dialysis (37 C, 30 min, 12-16 kDa) SIJ: 5 mL dialysis (37 C, 2 h, 12-16 kDa)	ICP OES	8
Baby foods	Cu, Fe, Mn, Zn	saliva: 8.96% (m/v) KCl 2.0% (m/v) KSCN 8.88% (m/v) NaH_2PO_4 5.7% (m/v) $NaSO_4$ 17.5% (m/v) NaCl 8.47% (m/v) $NaHCO_3$ 2.5% (m/v) urea 0.06% (m/v) α-amylase 0.003% (m/v) uric acid 0.005% (m/v) mucin gastric juice: 17.5% (m/v) NaCl 8.88% (m/v) NaH_2PO_4 8.96% (m/v) KCl 2.22% (m/v) $CaCl_2{\cdot}2H_2O$ 3.06% (m/v) NH4Cl, 37% (m/m) HCl 6.5% (m/v) glucose 0.2% (m/v) glucoronic acid 2.5% (m/v) urea 3.3% glucosamine hydrochloride 0.2% (m/v) BSA 0.2% (m/v) pepsin 0.6% (m/v) mucin	duodenal juice: 17.5% (m/v) NaCl 8.47% (m/v) $NaHCO_3$ 0.8% (m/v) KH_2PO_4 8.96% (m/v) KCl 0.5% (m/v) $MgCl_2$ 37% (m/m) HCl 2.22% (m/v) $CaCl_2{\cdot}2H_2O$ 2.5% (m/v) urea 0.2% (m/v) BSA 1.8% (m/v) pancreatin 0.3% (m/v) lipase bile juice: 17.5% (m/v) NaCl 8.47% (m/v) $NaHCO_3$ 8.96% (m/v) KCl 37% (m/m) HCl 2.22% (m/v) $CaCl_2{\cdot}2H_2O$ 2.5% (m/v) urea 0.36% (m/v) BSA 6% bile	sample: 3 g flour/baby food saliva (6/3 mL, 5 min, pH 6.8) SGJ: 12/6 mL (pH 2-3) incubation (37 °C, 2 h, shaking) --- pH 6.5-7 (1 mol L^{-1} HCO_3^-) SIJ: duodenal 12/6, bile 6/3 incubation (37 °C, 2 h, shaking) centrifugation (3600 rpm, 30 min) microwave mineralization of supernatant from gastrointestinal digestion: 5 mL of digest + 3 mL 65% (v/v) HNO_3 + 1 mL 30% (v/v) H_2O_2, 33 min final volume: 15 mL	ICP MS	9

Table S1. Conditions of the *in vitro* gastrointestinal digestion of different food samples (cont.)

Sample	Analyte	Simulated gastric juice (SGJ)	Simulated intestinal juice (SIJ)	Experimental details	Detection	Reference
Edible seaweed	As	6% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.4% (m/v) pancreatin + 2.5% (m/v) bile salt in 0.1 mol L^{-1} $NaHCO_3$	sample: 0.5 g + 20 mL H_2O pH 2.0 (6 mol L^{-1} HCl) SGJ: 0.15 g incubation (37 °C, 2 h, shaking) an ice-water bath - stopping the digestion SIJ: 5 mL pH 7.5 (20 mL 0.15 N PIPES solution) dialysis (37 °C, 2 h, shaking, 10 kDa) an ice-water bath - stopping the digestion	ICP MS	10
Fruit juices	Fe	4% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.02% (m/v) pancreatin + 1.2% (m/v) bile salt in 0.1 mol L^{-1} $NaHCO_3$	sample: 10 mL pH 2 (0.05 mol L^{-1} HCl) SGJ: 1 mL incubation (37 °C, 2 h, shaking) dialysis (20 mL PIPES buffer, 37 °C, 30 min, 6-8 kDa) SIJ: 5 mL dialysis (37 °C, 2 h, 6-8 kDa)	ICP OES	11
White cheese, bread, fruit, vegetables	Cu, Fe, Mn, Mo, Zn	1% (m/v) pepsin in 0.15 mol L^{-1} NaCl (pH 2.5)	3% (m/v) pancreatin + 1% amylase + 0.15% (m/v) bile salt	sample: 0.3 g SGJ: 10 mL incubation (37 °C, 4 h, shaking) pH 7.4 (1.0 mol L^{-1} NaOH) SIJ: 5 mL incubation (37 °C, 4 h, shaking) centrifugation (4000 rpm, 15 min)	DF-SP-ICP MS	12
Chocolate drink powder	Al, Ba, Cd, Cr, Cu, Mg, Mn, P	saliva: 0.18% (m/v) KCl 0.04% (m/v) KSCN 0.18% (m/v) NaH_2PO_4 0.11% (m/v) $NaSO_4$ 0.06% (m/v) NaCl 0.34% (m/v) $NaHCO_3$ 0.04% (m/v) urea 0.06% (m/v) α-amylase 0.003% (m/v) uric acid 0.005% (m/v) mucin gastric juice: 0.55% (m/v) NaCl 0.05% (m/v) NaH_2PO_4 0.16% (m/v) KCl 0.08% (m/v) $CaCl_2$ 0.06% (m/v) NH_4Cl, 1.3% (m/m) HCl 0.13% (m/v) glucose 0.004% (m/v) glucoronic acid 0.02% (m/v) urea 0.07% glucoseamine hydrochloride 0.2% (m/v) BSA 0.5% (m/v) pepsin 0.6% (m/v) mucin	duodenal juice: 0.14% (m/v) NaCl 0.67% (m/v) $NaHCO_3$ 0.016% (m/v) KH_2PO_4 0.11% (m/v) KCl 0.01% (m/v) $MgCl_2$ 0.04% (m/m) HCl 0.04% (m/v) $CaCl_2$ 0.02% (m/v) urea 0.2% (m/v) BSA 1.8% (m/v) pancreatin 0.3% (m/v) lipase bile juice: 1.05% (m/v) NaCl 1.16% (m/v) $NaHCO_3$ 0.08% (m/v) KCl 0.03% (m/m) HCl 0.04% (m/v) $CaCl_2$ 0.05% (m/v) urea 0.36% (m/v) BSA 6% bile	sample: 2.25 g saliva (1.5 mL, 5 min, pH 6.8) SGJ: 3 mL incubation (37 °C, 2 h, shaking) pH 6.5-7 (1 mol L^{-1} HCO_3^-) SIJ: duodenal 3 mL, bile 1.5 mL incubation (37 °C, 2 h, shaking) an ice-water bath - stopping the digestion centrifugation (2000 rpm, 30 min) microwave mineralization of supernatant from gastrointestinal digestion: 5 mL of digest + 3 mL 65% (v/v) HNO_3 + 1.5 mL 30% (v/v) H_2O_2 + 3.5 mL H_2O, 33 min final volume: 25 mL	ICP OES	13

Table S1. Conditions of the *in vitro* gastrointestinal digestion of different food samples (cont.)

Sample	Analyte	Simulated gastric juice (SGJ)	Simulated intestinal juice (SIJ)	Experimental details	Detection	Reference
Bee honeys	Ca, Cu, Fe, Mg, Mn, zn	0.32% (m/v) pepsin + 0.2% (m/v) NaCl in 0.08 mol L^{-1} HCl	1.0% (m/v) pancreatin + 1.25% (m/v) bile salt + 0.007% (m/v) K_2HPO_4 in 0.02 mol L^{-1} NaOH	sample: 2.5 g SGJ: 10 mL incubation (37 °C, 2 h, shaking) pH 7.0 (30 mg mL^{-1} $NaHCO_3$) SIJ: 10 mL incubation (37 °C, 2 h, shaking) H_2O (up 100 mL) ultrafiltration (5 kDa)	FAAS	14
Tea	Ca, Cu, Fe, Mg, Mn, K, Na, Zn	SGJ from patients undergoing routine upper gastrointestinal endoscopy	–	sample: tea infusion SGJ: 10 mL incubation (37 °C, 1 h, shaking) ultrafiltration (4000 g, 90 min, 3 kDa, 10 kDa, 30 kDa) pH 6.5 ($NaHCO_3$) incubation (37 °C, 24 h, shaking) ultrafiltration (3 kDa, 10 kDa, 30 kDa)	ICP OES	15
Human, cow, goat and sheep milk	Ca, Zn	16% (m/v) pepsin in 0.1 mol L^{-1} HCl	0.4% (m/v) pancreatin + 2.5% (m/v) bile salt in 0.1 mol L^{-1} $NaHCO_3$	sample: 100 g pH 2.0 (6 mol L^{-1} HCl) SGJ: 3 mL incubation (37 °C, 2 h, shaking) sample: 20 g gastric digest + 25 mL H_2O + $NaHCO_3$ (pH 7.5) dialysis (37 °C, 30 min, shaking, 10-12 kDa) SIJ: 5 mL dialysis (37 °C, 2 h, shaking, 10-12 kDa)	FAAS	16
Whole grain tea-biscuits	Ca, Cu, Mg, Mn	0.001% (m/v) pepsin in 0.02 mol L^{-1} HCl/NaCl (pH 2)	3.04% (m/v) pancreatin + 1% (m/v) amylase; 0.156% (m/v) bile salt	sample: 20 g SGJ: 100 mL incubation (37 °C, 3 h, shaking) pH 7.5 (6% $NaHCO_3$) SIJ: 20 mL + 20 mL incubation (37 °C, 2 h, shaking) filtration	ICP OES	17
"Zhebawei" herbal medicines	As, Cd, Cu, Fe, Mn, Zn	16% (m/v) pepsin in 0.1 mol L^{-1} HCl (pH 2)	0.4% (m/v) pancreatin + 2.5% (m/v) bile salt in 0.1 mol L^{-1} $NaHCO_3$	sample: 20 mL (decoction) pH 2 (HCl) SGJ: 5 mL incubation (37 °C, 50 min, shaking) pH 5.3 ($NaHCO_3$) SIJ: 8 mL pH 6.8-7.0 incubation (37 °C, 4h, shaking) centrifugation (5000 rpm, 20 min) filtration:(45 mm)	ICP OES	18

FAAS: flame atomic absorbtion spectroscopy; ETAAS: electrothermal atomic absorption spectrometry; GFASS: graphite furnace atomic absorption spectrometry; ICP OES: inductively coupled plasma optical emission spectrometry; ICP MS: inductively coupled plasma mass spectrometry; DF-SP-ICP MS: double focusing single particle inductively coupled plasma mass spectrometry; BSA: bovine serum albumin; PIPES: piperazine-*N*,*N*'-bis(2-ethanesulfonic acid).

Table S2. Calculated values of the Snedecor-Fisher *F*-test ($|F_{calculated}|$) and the paired t-test ($|t_{calculated}|$) for the comparison of percentage contributions of the soluble and the bioaccessible fractions of elements obtained using two different gastrointestinal solutions (SGJ1 + SIJ1 and SGJ2 + SIJ2). Significant differences between results are underlined

	Soluble fraction		Bioaccessible fraction	
	$F_{calculated}$	$t_{calculated}$	$F_{calculated}$	$t_{calculated}$
Ba	6.76	1.484	1.09	1.865
Ca	1.27	1.246	1.96	8.951
Cr	1.16	0.858	6.02	5.385
Cu	4.13	0.883	8.27	1.232
Fe	3.24	2.768	1.56	3.873
Mg	4.39	0.041	1.72	1.422
Mn	1.22	0.848	1.22	2.330
P	1.06	2.589	1.36	3.080
Sr	6.76	1.292	3.48	2.770
Zn	1.44	11.779	4.00	8.050

Critical value of the Snedecor-Fisher *F*-test ($F_{critical}$): 19.00 (p = 0.05); critical value of the paired *t*-test ($t_{critical}$): 2.447 (p = 0.05).

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