SUPPLEMENTARY INFORMATION

Bioaccessibility of Bioactive Compounds of 'Fresh Garlic' and 'Black Garlic' Through *In-Vitro* Gastrointestinal Digestion.

Alicia Moreno-Ortega[a,b], Gema Pereira-Caro[a*], José Luis Ordóñez[a], Rafael Moreno-Rojas[b], Víctor Ortíz-Somovilla[a], José Manuel Moreno-Rojas[a*]

[a]Department of Food Science and Health, Andalusian Institute of Agricultural and Fisheries Research and Training (IFAPA), Alameda del Obispo, Avda. Menéndez-Pidal, s/n. 14004, Córdoba, Spain

[b]Departamento de Bromatología y Tecnología de los Alimentos, Campus Rabanales, Ed. Darwin-anexo Universidad de Córdoba, 14071, Córdoba, Spain

*Corresponding authors:
Gema Pereira-Caro (mariag.pereira@juntadeandalucia.es)
José Manuel Moreno-Rojas (josem.moreno.rojas@juntadeandalucia.es)
IFAPA-Alameda del Obispo, Department of Food Science and Health, Avenida Menéndez Pidal, S/N, 14071 Córdoba (Spain). Tel. 0034 671 532 734

Table S1. Details of the Simulated Salivary Fluid (SSF), Simulated Gastric Fluid (SGF) and Simulated Intestinal Fluid (SIF)

	$MgCl_2(H_2O)_6$ (0.15 M)	KCl (0.5 M)	KH_2PO_4 (0.5 M)	$(NH_4)_2CO_3$ (0.5 M)	$NaHCO_3$ (1 M)	NaCl (2 M)	Distilled Water	Final Volume
					mL			
SSF	0.313	9.438	2.313	0.038	4.250	-	233.650	**250.0**
SGF	0.250	4.313	0.563	0.313	7.813	7.375	229.375	**250.0**
SIF	0.688	4.250	0.500	0.688	26.563	6.000	211.313	**250.0**

Table S2. HPLC-HRMS-Based Identifications of (Poly)phenols in Fresh and Black Garlics

Peak	RT	Compound	Chemical Formula $[m/z]^-$	Experimental Mass $[m/z]^-$	δ (ppm)	MSI MI level[a]
1	4.7	Epigallocatechin	C15H13O7	305.066	-0.48	2
2	7.2	Benzoic Acid	C7H5O2	121.028	0.68	1
3	8.0	Chlorogenic acid	C16H17O9	353.087	-1.13	1
4	8.2	Catechin	C15H13O6	289.071	-1.09	1
5	8.3	Caffeic acid	C9H7O4	179.034	0.28	1
6	9.7	Gallic acid	C7H5O5	169.013	-2.15	1
7	11.7	Epicatechin	C15H13O6	289.071	-1.09	1
8	18.9	Vanillic acid	C8H7O4	167.034	0.67	2
9	21.1	Ferulic acid	C10H9O4	193.050	1.79	1
10	24.4	*p*-Coumaric acid	C9H7O3	163.039	-1.96	1

[a]Metabolite standards initiative (MSI) metabolite identification (MI) levels [1]. Reference compounds were available for all compounds identified at MSI MI level 1

Table S3. HPLC-HRMS-Based Identifications of organosulfur compounds in Fresh and Black Garlics

Peak	RT	Compound	Chemical Formula $[m/z]^+$	Experimental Mass $[m/z]^+$	δ (ppm)	MSI MI level[a]
1	4.2	S-Allylmercapto-L-cysteine (SAMC)	C6H12NO2S2	194.030	0.85	2
2	4.6	S-Allylcysteine (SAC)	C6H12NO2S	162.058	-1.9	1
3	5.7	S-Methylcysteine (Deoxymethiin)	C4H10NO2S	136.043	0.11	2
4	5.8	S-Propyl-L-cysteine sulfoxide (Propiin)	C6H14NO3S	180.069	2.45	2
5	5.9	S-(S-propyl) cysteine	C6H14NO2S2	196.046	0.36	2
6	5.9	Cycloalliin	C6H12NO3S	178.053	-1.36	2
7	6.6	γ –Glutamyl-S-(S-1-propenyl) cysteine (GS1PC)	C11H19N2O5S	291.101	1.65	2
8	6.7	γ-Glutamyl-S-allylmercaptocysteine (GSAMC)	C11H19N2O5S2	323.073	-1.9	2
9	6.8	S-Allylsulfenic acid (Lacrimatory factor)	C3H7OS	91.021	3.42	2
10	6.8	N-Acetyl-S-allyl-L-cysteine (NASAC)	C8H14NO3S	204.069	-1.39	2
11	6.8	Alliin	C6H12NO3S	178.053	-2.82	1
12	6.8	γ –Glutamyl-S-(S-1-propenyl)cysteine-glycine	C13H22N3O6S2	380.094	0.92	2
13	7.0	S-(2-carboxypropyl) cysteine	C7H14NO4S	208.064	-2.15	2
14	7.1	Trans-S-(1-propenyl)-L-cysteine (S1PC)	C6H12NO2S	162.058	-0.70	2
15	7.3	γ −Glutamyl-S-allyl-L-cysteine (GSAC)	C11H19N2O5S	291.101	1.86	2
16	7.4	S-Allylglutathione	C13H22N3O6S	348.122	-0.23	2
17	7.6	S-Methyl-l-cysteine sulfoxide (Methiin)	C4H10NO3S	152.038	-1.33	2
18	7.6	γ –Glutamyl-S-(S-methyl)cysteine-glycine	C11H20N3O6S2	354.079	-0.51	2
19	7.7	Methionine sulfoxide	C5H11NO3S	166.053	1.94	2
20	8.5	γ -Glutamyl-cysteine	C8H15N2O5S	251.070	-2.45	2
21	8.6	γ –Glutamyl-S-(2-carboxypropyl)cysteine-glycine	C14H24N3O8S	394.128	0.67	2
22	9.0	γ-Glutamyl-S-(1-propenyl) cysteine sulfoxide (G1PCS)	C11H19N2O6S	307.096	-2.05	2
23	9.2	ɣ-Glutamyl-S-methyl-L-cysteine (GSMC)	C9H17N2O5S	265.085	1.56	2
24	10.0	ɣ −Glutamyl-S-methyl-L-cysteine sulfoxide (GSMCS)	C9H17N2O6S	281.080	2.19	2

[a]Metabolite standards initiative (MSI) metabolite identification (MI) levels [1]. Reference compounds were available for all compounds identified at MSI MI level 1

References

1. Sumner, L.W.; Amberg, A.; Barrett, D.; Beale, M.H.; Beger, R.; Daykin, C.A.; W-M Fan, T.; Fiehn, O.; Goodacre, R.; Griffin, J.L.; et al.

Proposed minimum reporting standards for chemical analysis Chemical Analysis Working Group (CAWG) Metabolomics Standards Initiative (MSI) *NIH Public Access. Metabolomics* **2007**, *3*, 211–221, doi:10.1007/s11306-007-0082-2.