SUPPLEMENTARY INFORMATION

Effect of colonic fermentation on the stability of fresh and black onion bioactives

Alicia Moreno-Ortega[1,2], Giuseppe Di Pede[3], Pedro Mena[3,4], Luca Calani[3], Daniele Del Rio[3,4], José Manuel Moreno-Rojas [2,5*], Gema Pereira-Caro[2,5*]

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

[2]Foods for Health Group, Instituto Maimónides de Investigación Biomédica de Córdoba (IMIBIC), Córdoba, Spain.

[3]Department of Food and Drugs, University of Parma, 43124 Parma, Italy;

[4]Microbiome Research Hub, University of Parma, 43124 Parma, Italy.

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

*Corresponding authors:

Dra. Gema Pereira-Caro (mariag.pereira@juntadeandalucia.es)

Dr. José Manuel Moreno-Rojas (josem.moreno.rojas@juntadeandalucia.es)

IFAPA-Alameda del Obispo, Department of Food Science and Health, Avenida Menéndez Pidal, SN, 14071 Córdoba (Spain). Tel. 0034 671 532 734

Table S1.- UHPLC-LIT-MS^n-based identification of phenolic and organosulfur compounds detected in fresh and black onion during in vitro colonic fermentation

Compound	RT (min)	Parent mass *(m/z)*	MS fragmentation pattern from full scan data dependent analyses (*m/z*)	MS^2 fragmentation pattern from full MS/MS analyses (*m/z*)	MSI MI Level*	Sample
Phenolic Compounds		**[M-H]$^-$**				
Flavonols						
Quercetin	6.12	301		**179**, 151, 273, 257, 193, 239, 107, 283	1	FO; BO
Kaempferol	6.97	285		**151**, 229, 257, 213, 243, 185, 169, 107, 143	1	FO; BO
Quercetin-3-*O*-rutinoside (rutin)	4.29	609		**301**, 300, 343, 271, 179, 591	1	FO; BO
Isorhamnetin	9.13	315		**297**, 279, 171, 241, 227, 151	2	FO; BO
Quercetin-3-*O*-glucoside	5.20	463		**301**, 343, 419, 373	2	FO; BO
Quercetin-4-*O*-glucoside	4.20	463		**373**, 351, 419, 342, 445, 301, 217	2	FO
Isorhamnetin glucoside	5.15	477		**315**, 396, 459, 357, 260, 408	2	FO
Flavone						
Luteolin	6.13	285		**241**, 175, 199, 217, 241, 257, 151, 107	1	FO; BO
Hydroxycinnamic acids						
4′-Hydroxycinnamic acid	3.31	163		**119**, 135	1	FO; BO
3′,4′-Dihydroxycinnamic acid	2.51	179		**135**, 151, 117, 91	1	FO; BO
4′-Hydroxy-3′-methoxycinnamic acid	3.70	193		**149**, 178, 134, 107	1	FO; BO
Phenylpropanoic acids derivatives						
3-(3′,4′-Dihydroxyphenyl)propanoic acid	1.85	181		**137**, 119, 59, 163	1	FO; BO
3-(4′-Hydroxy-3′-methoxyphenyl)propanoic acid	3.08	195		**136**, 151, 177, 123, 59	1	FO; BO
3-(3′-Hydroxy-4′-methoxyphenyl)propanoic acid	3.42	195		**119**, 151,149, 136, 180, 93	1	BO
3-(3′-Hydroxyphenyl)propanoic acid	3.10	165		**121**, 147, 165, 97	1	FO; BO
3-Phenylpropanoic acid	4.80	149		**105**, 131	1	FO; BO
Phenylacetic acids derivatives						
4′-Hydroxyphenylacetic acid	1.85	151		**107**, 120, 93	1	FO; BO
3-Phenylacetic acid	3.36	135		**91**	1	BO

Benzoic acids derivatives						
Benzoic acid	3.50	121		**77**	1	FO; BO
4-Hydroxy-3-methoxybenzoic acid	2.31	167		**123**, 152, 108, 79	1	FO; BO
3,4-Dihydroxybenzoic acid	1.16	153		**109**, 135, 81	1	FO; BO
3-Hydroxybenzoic acid	2.08	137		**93**, 115	1	FO; BO
4-Hydroxybenzoic acid	1.78	137		**93**	1	FO; BO
3-Hydroxy-4-methoxybenzoic acid	2.44	167		**152**, 123, 99	1	FO; BO
3,4,5-Trihydroxybenzoic acid	0.74	169		**125**, 97, 81	1	BO
Hydroxycarboxilic acids derivatives						
3′-Hydroxymandelic acid	0.87	167		**123**, 105, 85	1	FO; BO
Benzenetriol						
Benzene-1,3,5-triol	0.65	125		**83**, 57	1	FO; BO
Organosulfur Compounds		**[M-H]$^+$**				
γ-Glutamyl-S-Alk(en)yl-L-Cysteine Sulfoxides						
γ −Glutamyl-*S*-methyl-*L*-cysteine sulfoxide (GSMCS)	4.85	281	**121**, 132, 173, 207, 235, 245		2	FO; BO
γ −Glutamyl-*S*-(2-propenyl) cysteine sulfoxide (G2PCS)	3.89	307	**229**, 269, 171, 146, 130		2	FO
γ −Glutamyl-*S*-(1-propenyl) cysteine sulfoxide (G1PCS)	7.92	307	**176**, 207, 134, 235, 269		2	FO; BO
γ-Glutamyl-S-Alk(en)yl-L-Cysteine Derivatives						
γ −Glutamyl-*L*-cysteine	4.06	251		**223, 2**34, 166, 178, 110, 206, 138	2	FO; BO
γ −Glutamyl-*S*-(S-methyl) cysteine-glycine	4.59	354	**244**, 118, 145, 260, 203		2	FO; BO
γ −Glutamyl-*S*-(2-carboxypropyl) cysteine-glycine	7.06	394	**148**, 365, 218, 291, 263		2	FO
γ −Glutamyl-*S*-allyl-L-cysteine (GSAC)	6.19	291		**162**, 145, 170, 274, 245, 122, 84	1	FO; BO
γ -Glutamyl-*S*-(2-propenyl) cysteine (GS2PC)	7.09	291	**148**, 291, 365, 203		2	FO; BO
γ −Glutamyl-*S*-(2-carboxypropyl) cysteine	6.95	335	**120**, 161, 203, 229, 290, 302		2	BO
S-Alk(en)yl-L-Cysteine Sulfoxides Derivatives						
Isoalliin	6.86	178		**88**, 91, 116, 73, 132, 160	2	FO; BO
Methionine sulfoxide	4.70	166		**121**, 149, 131	2	FO; BO
S-propyl-*L*-cysteine sulfoxide (Propiin)	8.68	180		**162**, 144, 134		BO
S-Alk(en)yl-L-Cysteine Derivatives						
S-Allylcysteine (SAC)	4.50	162		**145**, 115, 134, 76, 99	1	FO; BO

S-Allylmercapto-*L*-cysteine (SAMC)	3.92	194	**171**, 154, 130, 136, 118	2	FO
S-Propyl-*L*-cysteine (Deoxypropiin)	9.38	164	**103**, 122, 132, 146	2	FO
S-Propylmercapto-*L*-cysteine (SPMC)	3.78	196	**104**, 171, 145, 110, 130, 184	2	FO; BO
S-(2-carboxypropyl) cysteine-glycine	6.95	265	**120**, 161, 230, 171, 244, 258	2	FO
S-(2-Carboxypropyl) cysteine	5.96	208	**105**, 171, 182, 132, 118, 146, 159	2	BO
S-Allylglutathione (SAG)	4.69	348	**229**, 203, 244, 105, 118, 270	2	BO

**Metabolite standards initiative (MSI) metabolite identification (MI) levels[31]. Reference compounds were available for all compounds identified at MSI MI level 1. RT: Retention time; m/z = mass to charge ratio; quantifier ions are reported in bold; FO: Fresh Onion; BO; Black Onion. Compounds for which there was a reference compound were quantified with them, while for the rest, the most structurally similar reference compound was used. Isorhamnetin was quantified with quercetin. γ-Glutamyl-S-Alk(en)yl-L-Cysteine Sulfoxides and γ-Glutamyl-S-Alk(en)yl-L-Cysteine were quantified with GSAC; Isoalliin was quantified with Alliin and Propiin with Methiin. S-Alk(en)yl-L-Cysteine were quantified with SAC.*