

TITTLE: Bioaccessibility of Tudela artichokes (*Cynara Scolymus* cv. Blanca de Tudela) (poly)phenols: effect of heat treatment, simulated gastrointestinal digestion and human colonic microbiota

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Table S1. Concentrations of electrolytes in Simulated Salivary Fluid (SSF), Simulated Gastric Fluid (SGF) and Simulated Intestinal Fluid (SIF). Final C is referred to the final concentration in the digestive fluid.

Compuesto	PM	Stock solution			SSF (250 mL)		SGF (250 mL)		SIF (250 mL)	
		g/mol	mol/L	g/L	g/50mL	Final C (mmol/L)	mL stock	Final C (mmol/L)	mL stock	Final C (mmol/L)
KCl	74.55	0.5	37.28	1.86	15.10	10.79	6.90	4.60	6.80	6.18
KH ₂ PO ₄	136.09	0.5	68.04	3.40	3.70	2.64	0.90	0.60	0.80	0.73
NaHCO ₃	84.01	1	84.01	4.20	13.60	4.86	25.00	8.33	85.00	38.64
NaCl	58.40	2	116.80	5.84	-	-	47.20	7.87	38.40	8.73
MgCl ₂ (H ₂ O) ₆	203.21	0.15	30.48	1.52	0.15	0.36	0.10	0.22	0.33	1.00
(NH ₄) ₂ CO ₃	96.09	0.5	48.05	2.40	0.06	0.04	0.50	0.33	-	-

Table S2. Mass spectrometric characteristics of (poly)phenolic compounds identified by LC-MS/MS

Compound	Rt (min)	[M-H] ⁻	MS/MS fragmentation	CE (eV)	LOQ (ng/L)	LOD (ng/L)
1-CQA	0.93	353	191(100), 179(3)	-20		-
3-CQA	1.45	353	191(100), 179(72)	-20		-
4-CQA	3.60	353	179(100), 179(90)	-25		-
5-CQA	3.19	353	191(100), 179(2)	-20	0.30	0.10
5-CQAcis	6.08	353	191(100), 173(1)	-20		-
Feruloyl-CQA	8.38	529	161(100), 367(40)	-40		-
1,3-diCQA	5.04	515	353(100), 191(83)	-30		-
1,4-diCQA	6.31	515	353(100), 173(38)	-25		-
3,4-diCQA	6.45	515	353(100), 173(88)	-30		-
1,5-diCQA	6.70	515	191(100), 353(35)	-30		-
3,5-diCQA	6.80	515	353(100), 191(67)	-30		-
4,5-diCQA	7.68	515	353(100), 173(56)	-30		-
diCQA glucoside I	6.10	677	191(100), 323(63)	-40		-
diCQA glucoside II	6.17	677	323(100), 515(96)	-40		-
Caffeoyl-hexoside	2.81	341	179(100), 135(32)	-30		-
Caffeic acid	3.22	179	135(100)	-30		-
Caffeic acid derivative	5.56	367	179(100), 135(44)	-30		-
p-coumaroylquinic acid I	4.32	337	191(100), 163(5)	-20		-
p-coumaroylquinic acid II	7.97	337	191(100), 163(45)	-20		-
Isoferulic acid	7.02	193	161(100), 134(96)	-35		-
Rutin	5.9	609	301(100)	-40	2.06	0.68
Apigenin 7-O-rutinoside	6.75	577	269(100)	-40		-
Apigenin 7-O-glucoside	7.22	431	269(100)	-50		-
Apigenin 7-O-glucuronide	6.08	445	269(100)	-30		-
Apigenin	10.45	269	117(100)	-40		-
Apigenin acetylglucoside	8.61	473	269(100)	-50		-
Luteolin 7-O-rutinoside	5.97	593	285(100)	-50		-
Luteolin 7-O-glucoside	6.08	447	285(100)	-40		-
Luteolin 7-O-glucuronide	6.10	461	285(100)	-30		-
Luteolin acetylglucoside	7.65	489	285(100)	-40		-
Luteolin	9.13	285	133(100),155(1)	-50		-
Pinoresinol 4-O-β-D-glucoside	6.41	519	357(100), 151(27)	-30		-
Pinoresinol-acetylhexoside	8.14	561	357(100)	-20		-
Dihydrocaffeic acid	2.94	181	59(100), 138(28)	-25	0.88	0.29
3-(3'-Hydroxyphenyl) propionic acid	5.15	165	121(100), 42(42)	-16	0.79	0.26
3-Phenylpropionic acid	8.36	149	105(100)	-15	52.6	17.4*
Phenylacetic acid	5.98	135	91(100)	-10	15.6	5.15
Dihydrocaffeoylquinic acid	1.21	355	181(100), 191(10)	-20		-
3',4'-dihydroxyphenylacetic acid	1.36	167	123(100)	-15	1.79	0.59
3'-hydroxyphenylacetic acid	3.59	151	107(100), 93(11)	-10	10.3	3.41
Protocatechuic acid	1.16	153	109(100), 81(3)	-20	0.21	0.07
1,2-Dihydroxybenzene (Catechol)	1.56	109	108(100),91(21)	-25	0.67	0.22
4-hydroxybenzoic acid	2.02	137	93(100)	-12	20.8	6.87

Rt, retention time; m/z, mass-to-charge ratio; [M-H]⁻, Negatively charged molecular ion; LOQ, limit of quantification of the standards used for quantification, LOD, limit of detection; *expressed as ng/mL

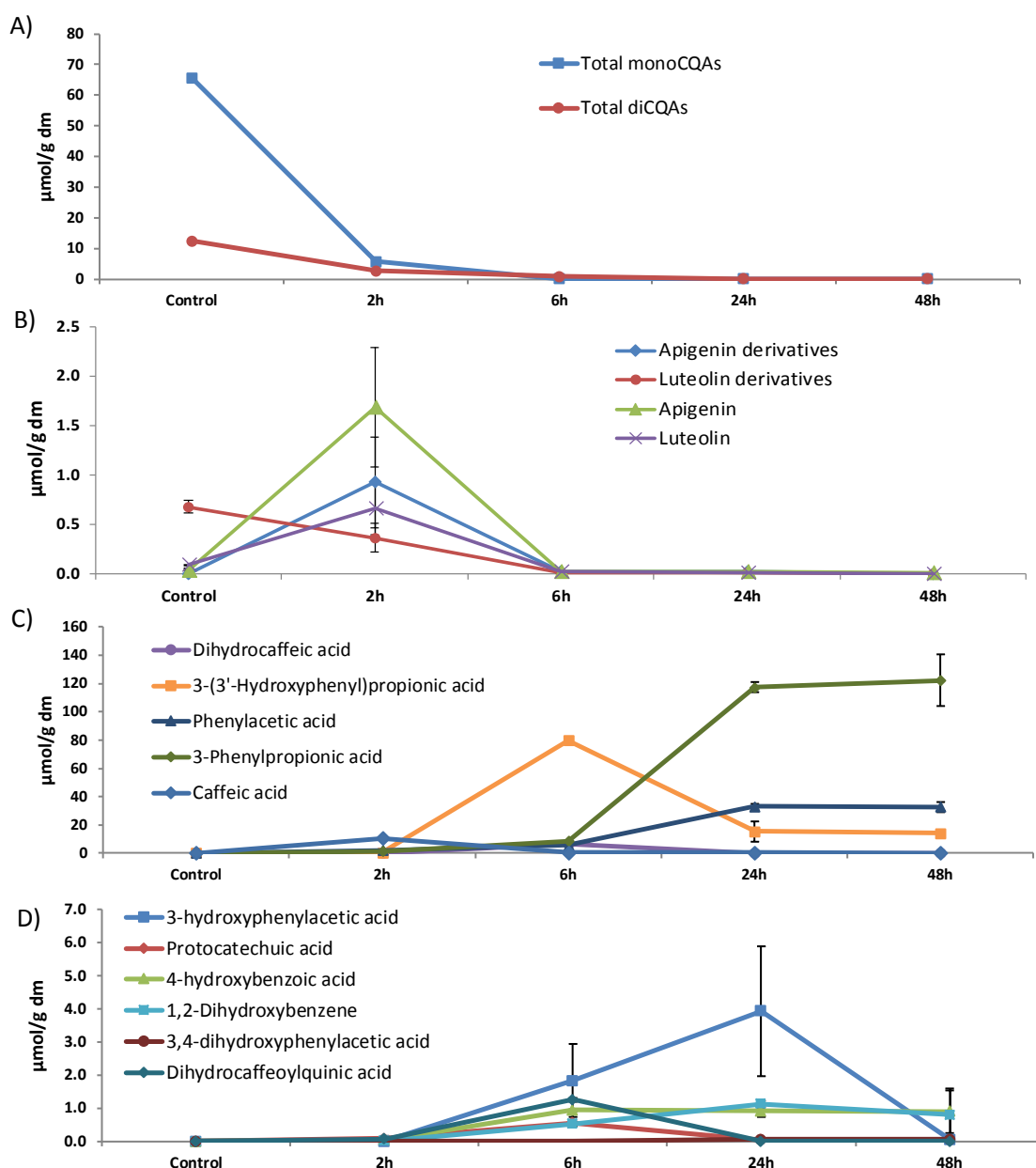


Figure S1. Profiles of degradation of native phenolic compounds of boiled artichokes and their catabolites during 48 h fecal fermentation. (A) Degradation of native phenolic acids: total monoCQAs and total diCQAs. (B) Degradation of native flavonoids. (C) Profile of the mayor phenolic catabolites produced. (D) Profile of the minor phenolic catabolites produced.

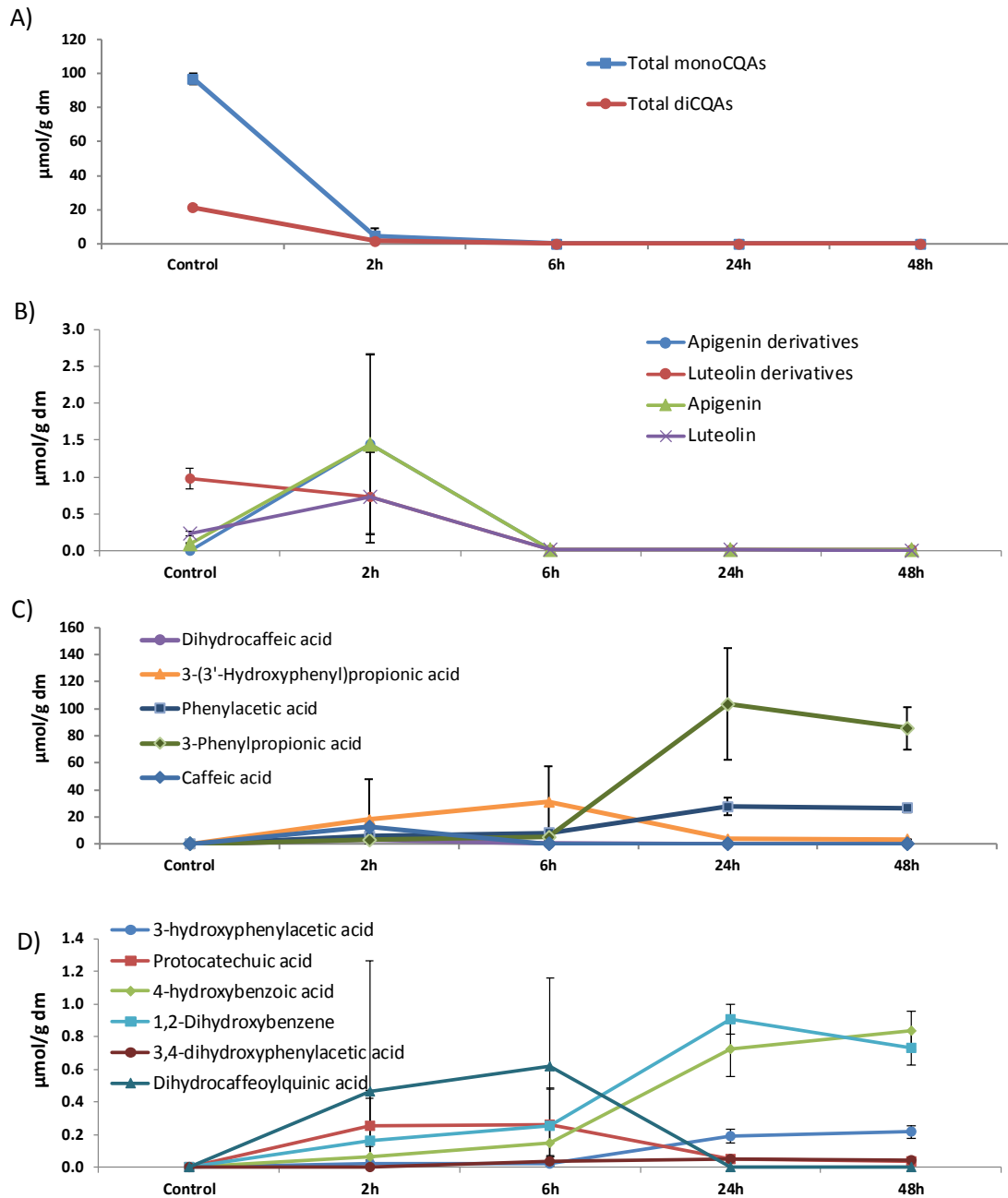


Figure S2. Profiles of degradation of native phenolic compounds of microwaved artichokes and their catabolites during 48 h fecal fermentation. (A) Degradation of native phenolic acids: total monoCQAs and total diCQAs. (B) Degradation of native flavonoids. (C) Profile of the mayor phenolic catabolites produced. (D) Profile of the minor phenolic catabolites produced.

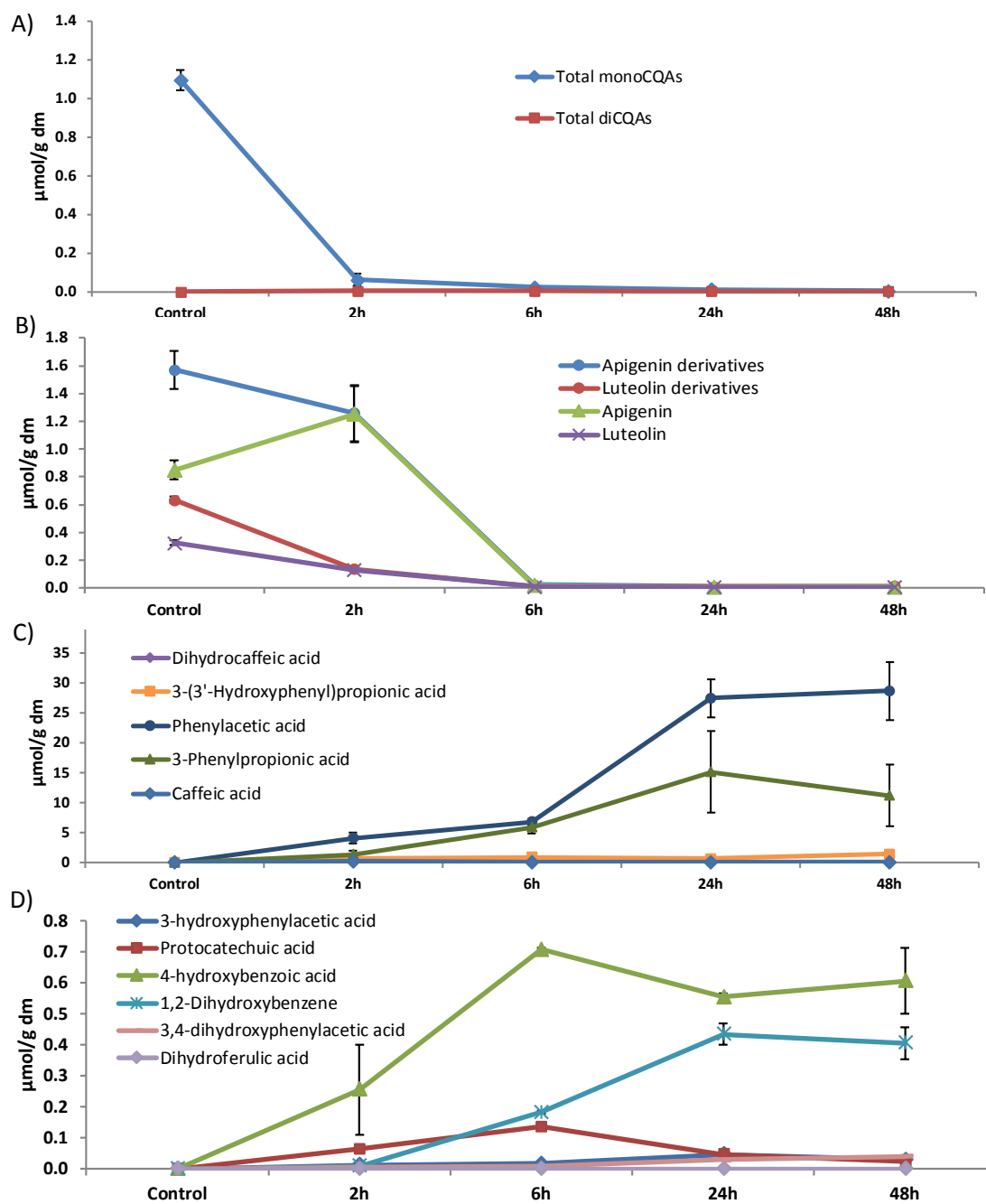


Figure S3. Profiles of degradation of native phenolic compounds of raw artichokes and their catabolites during 48 h fecal fermentation. (A) Degradation of native phenolic acids: total monoCQAs and total diCQAs. (B) Degradation of native flavonoids. (C) Profile of the mayor phenolic catabolites produced. (D) Profile of the minor phenolic catabolites produced.