A dynamic view on the chemical composition and bioactive properties of mulberry fruit during *in-vitro* digestion and fermentation model

Dou Zu-Man [a,b], Chen Chun [a, b, c]*, Fu Xiong [a,b,d,e] **, Liu Rui-Hai [a,f]

[a] School of Food Science and Engineering, South China University of Technology, 381 Wushan Road, Guangzhou 510640, China

[b] SCUT-Zhuhai Institute of Modern Industrial Innovation, Zhuhai 519715, China

[c] Guangzhou Institute of Modern Industrial Technology, Nansha, 511458, China

[d] Guangdong Province Key Laboratory for Green Processing of Natural Products and Product Safety, Guangzhou 510640, China

[e] Overseas Expertise Introduction Center for Discipline Innovation of Food Nutrition and Human Health (111 Center), Guangzhou 510640, China

[f] Department of Food Science, Stocking Hall, Cornell University, Ithaca, NY, 14853, USA

Corresponding author

*Chun Chen: chenc@scut.edu.cn

**Xiong Fu: lfxfu@scut.edu.cn

Table S1. Molecular interactions between α-glucosidase and major free phenolics released during the digestion.

Phenolics	Binding energy (Kcal/mol)	Number of binding to residues	Conventional hydrogen bond	Carbon hydrogen bond	Pi-Anion	Pi-Sigma	Pi-Alkyl	Pi-Pi T-shaped	Pi-Cation	Unfavorable Donor-Donor
2,4,6-trihydroxybenzoic acid	-2.92	3	Pro 312	Arg 315	Asp 307	Pro 312	-	-	-	-
cyanidin-3-O-glucoside	-7.77	6	Glu 411, Pro 312, Asp 242, Ser 240	Asp 242, Pro 312	Asp 307	-	Arg 315	-	-	-
3,4-dihydroxybenzoic acid	-3.19	3	Thr 310, Asp 307	-	-	-	Val 308	-	-	-
gallic acid	-3.67	10	Gln 279, Glu 277, Arg 213, Asp 215, Asp 69	-	Asp 352, Arg 442	-	Val 216	Tyr 72	Asp 215	His 351

Table S2. The community compositions (%) of intestinal microbiota at phylum level among different treatment groups.

Treatment	Time (h)	Pyhlum [a]			
		Firmicutes	Bacteroidetes	Proteobacteria	Actinobacteria
Initial	0	81.46±1.35a	6.18±0.41f	11.10±0.44e	1.20±0.21a
Blank	12	65.53±1.28b	21.78±0.76e	12.28±0.49d	0.40±0.01c
	24	43.00±1.02d	21.75±0.67e	34.87±0.87b	0.37±0.02c
Mulberry	12	23.53±0.53f	52.51±0.94a	23.59±0.62c	0.32±0.05d
	24	22.55±0.49f	33.93±0.71d	42.84±0.94a	0.64±0.08b
Inulin	12	45.31±0.86c	49.3±0.89b	5.24±0.41f	0.16±0.01f
	24	40.77±0.78e	46.19±0.87c	12.82±0.52d	0.21±0.01e

[a] Values in the same line with different lowercase letters means significant difference ($p < 0.05$), and data are expressed as the mean ± standard deviation (SD).

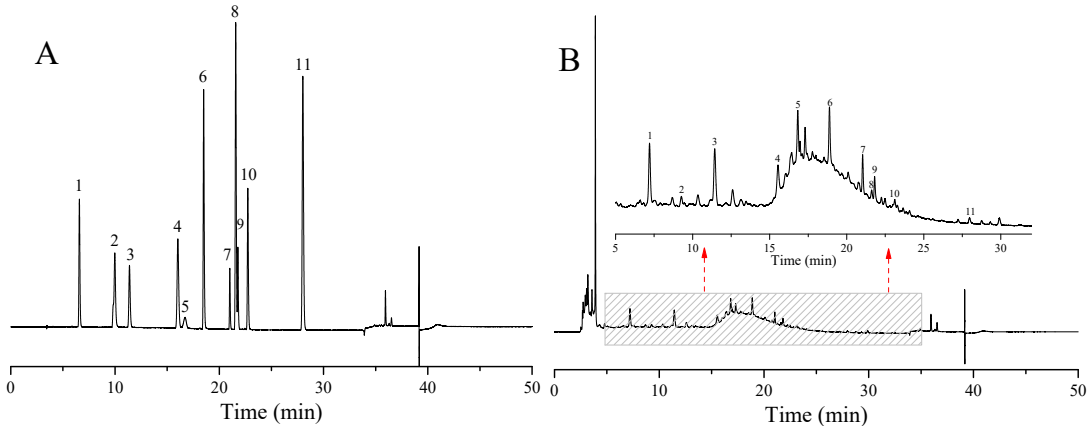

Fig. S1. Representative chromatograms determined by HPLC-DAD method. (A) standard phenolic mixture; (B) water alcohol extract of mulberry fruit. Peaks: 1, gallic acid; 2, 2,4,6-trihydroxybenzoic acid; 3, 3,4-dihydroxybenzoic acid; 4, catechol; 5, cyanidin-3-O-glucoside; 6, caffeic acid; 7, rutin; 8, p-coumaric acid; 9, quercetin-3-O-glucoside; 10, ferulic acid; 11, coumarin.

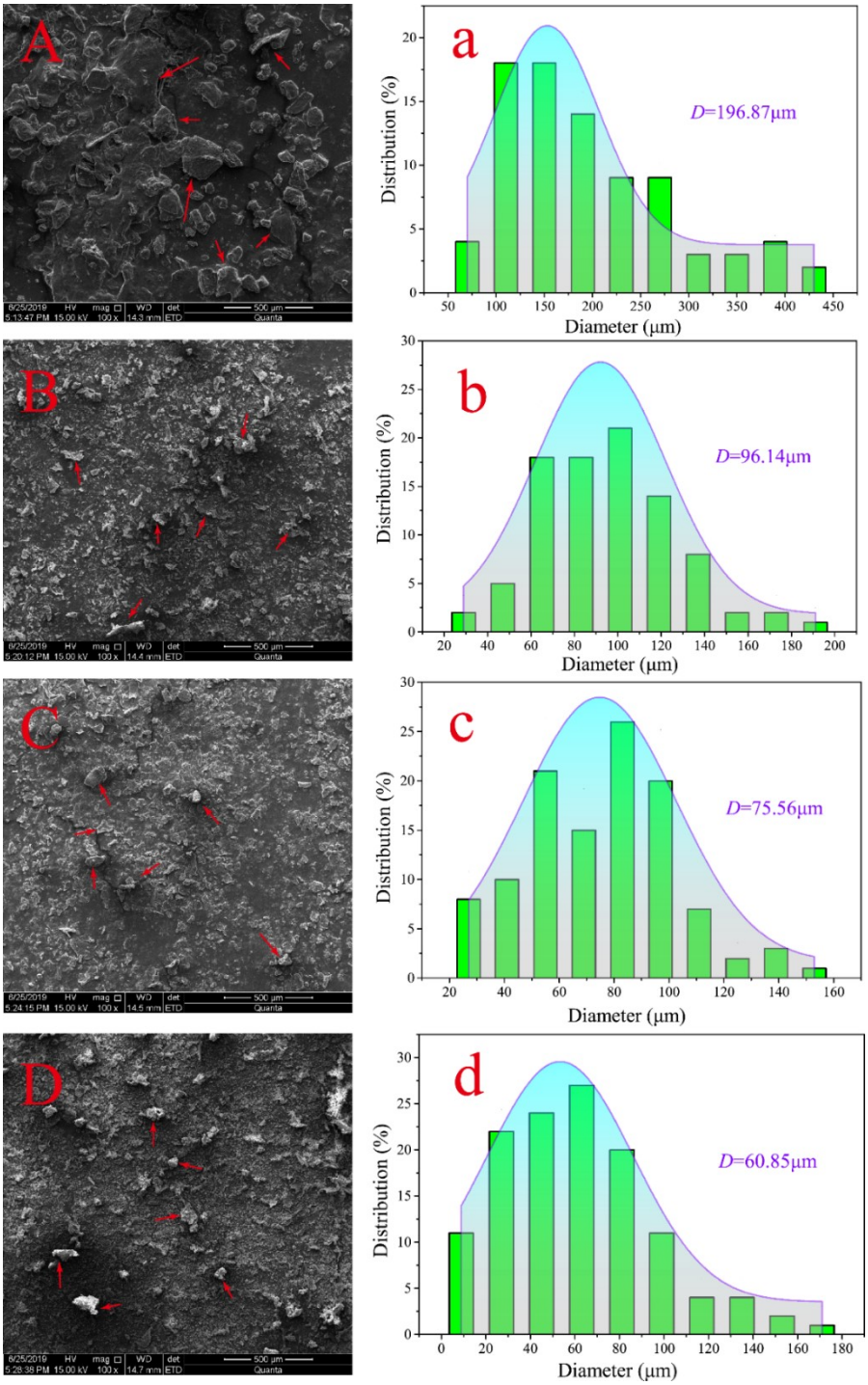

Fig. S2. The scanning electron micrographs (SEM) of undigested sample (A), oral (B), gastric (C) and intestine (D) digested fractions of mulberry fruit with magnification of 100 × . The corresponding particle size statistic analysis of undigested sample (a), oral (b), gastric (c) and intestine (d) digested fractions of mulberry fruit, respectively.

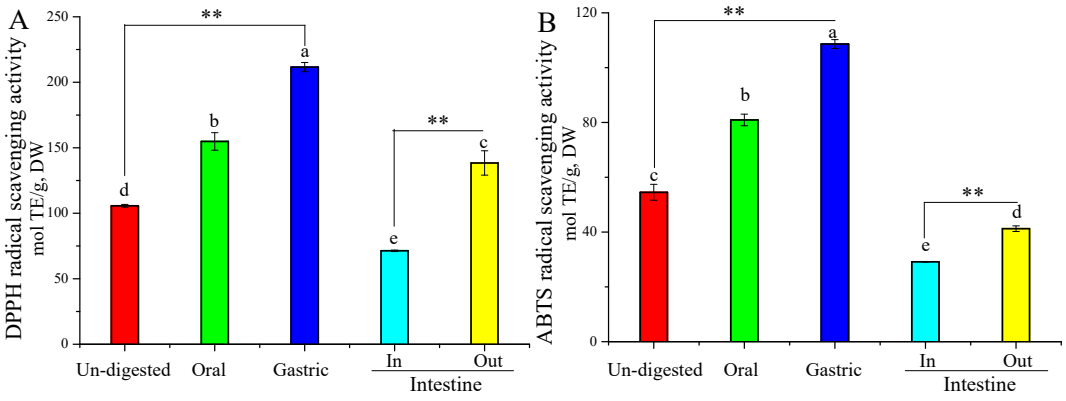

Fig. S3. Antioxidant activity of undigested samples and digested fractions of mulberry fruits. (A) the DPPH radical scavenging activity; (B) the ABTS radical scavenging activity. Un-digested samples were extracted with 80% ethanol (v/v).

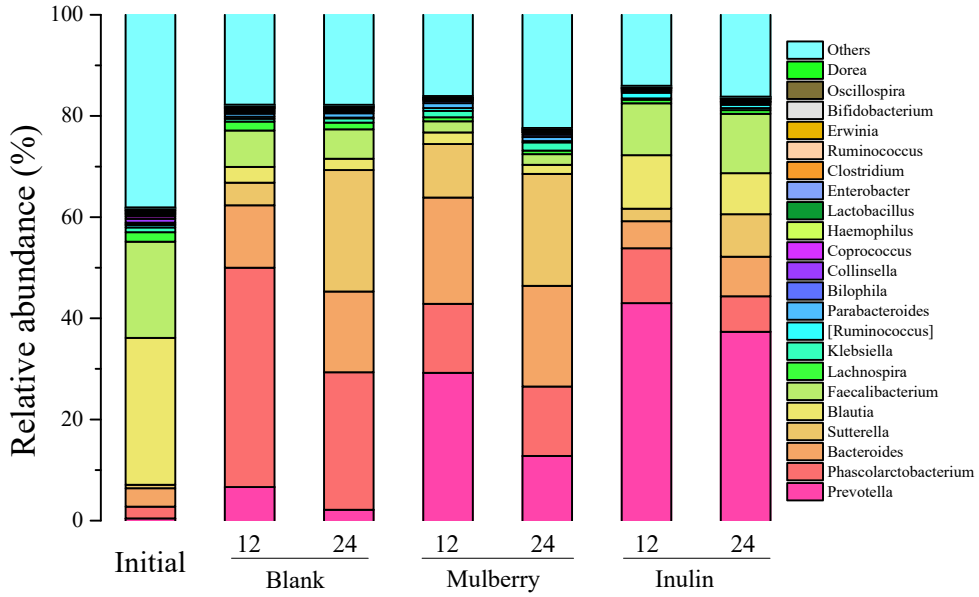

Fig. S4. The average relative abundance of microbial community at genus level.