foods

Effect of simulated gastrointestinal digestion on the phenolic composition and bioactivity of *Cymbopogon flexuosus* extracts

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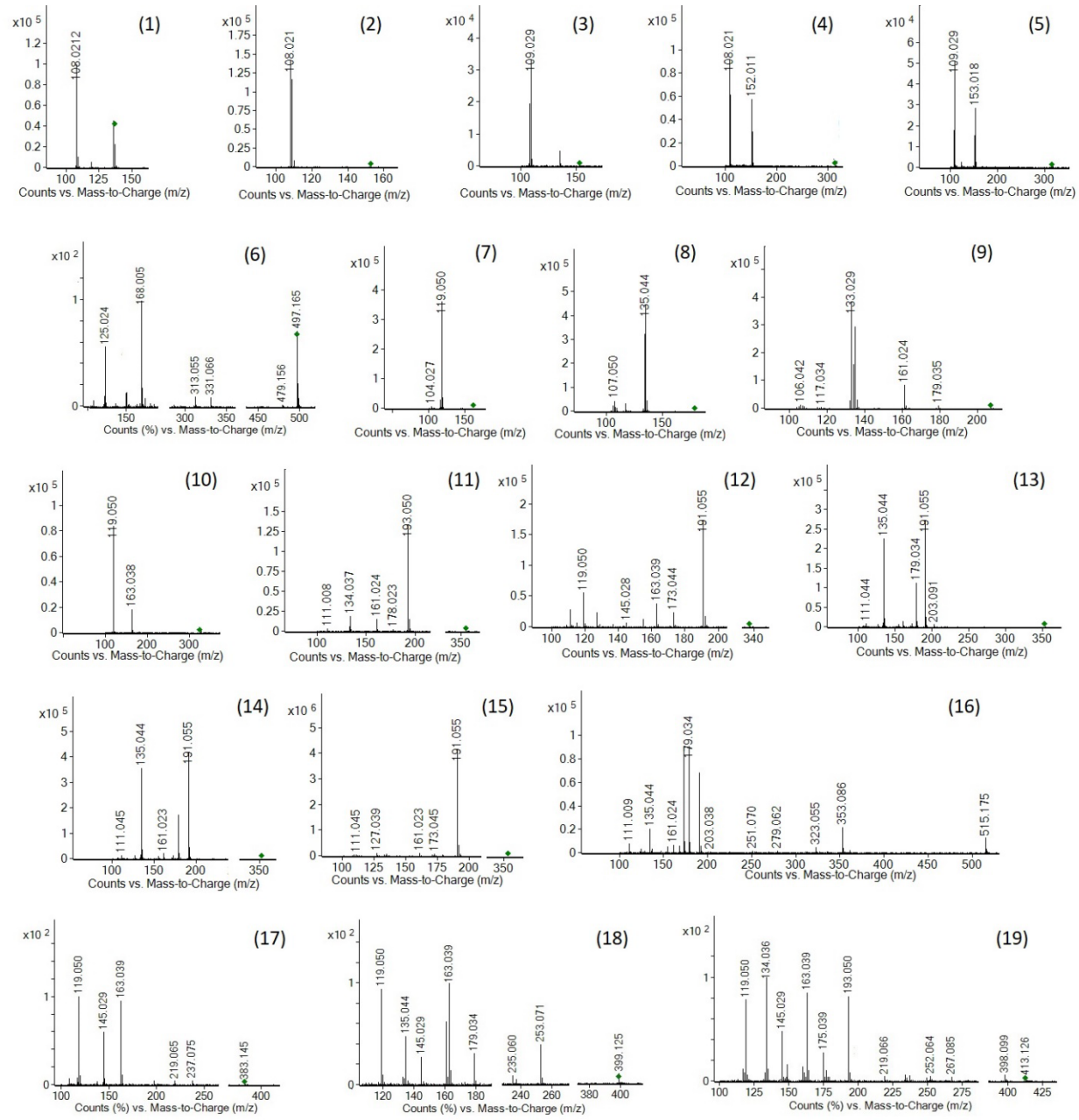


Figure S1. Fragmentation patterns (MS/MS spectra) of identified phenolic acids and derivatives: (**1**) Hydroxybenzoic acid; (**2**) Dihydroxybenzoic acid is. I (Protocatehuic acid); (**3**) Dihydroxybenzoic acid is. II (Gentisic acid); (**4**) Dihydroxybenzoic acid hexoside is. I; (**5**) Dihydroxybenzoic acid hexoside is. II; (**6**) Globulsin B; (**7**) Coumaric acid; (**8**) Caffeic acid; (**9**) Ethyl caffeate; (**10**) Coumaric acid hexoside; (**11**) Ferulic acid hexoside; (**12**) Coumaroylquinic acid; (**13**) Caffeoylquinic acid is. I; (**14**) Caffeoylquinic acid is. II; (**15**) Caffeoylquinic acid is. III (Chlorogenic acid); (**16**) Dicaffeoylquinic acid; (**17**) 1,3-*O*-Dicoumaroyl-glycerol; (**18**) 1,3-*O*-Coumaroyl-caffeoyl-glycerol; (**19**) 1,3-*O*-Coumaroyl-feruloyl-glycerol.

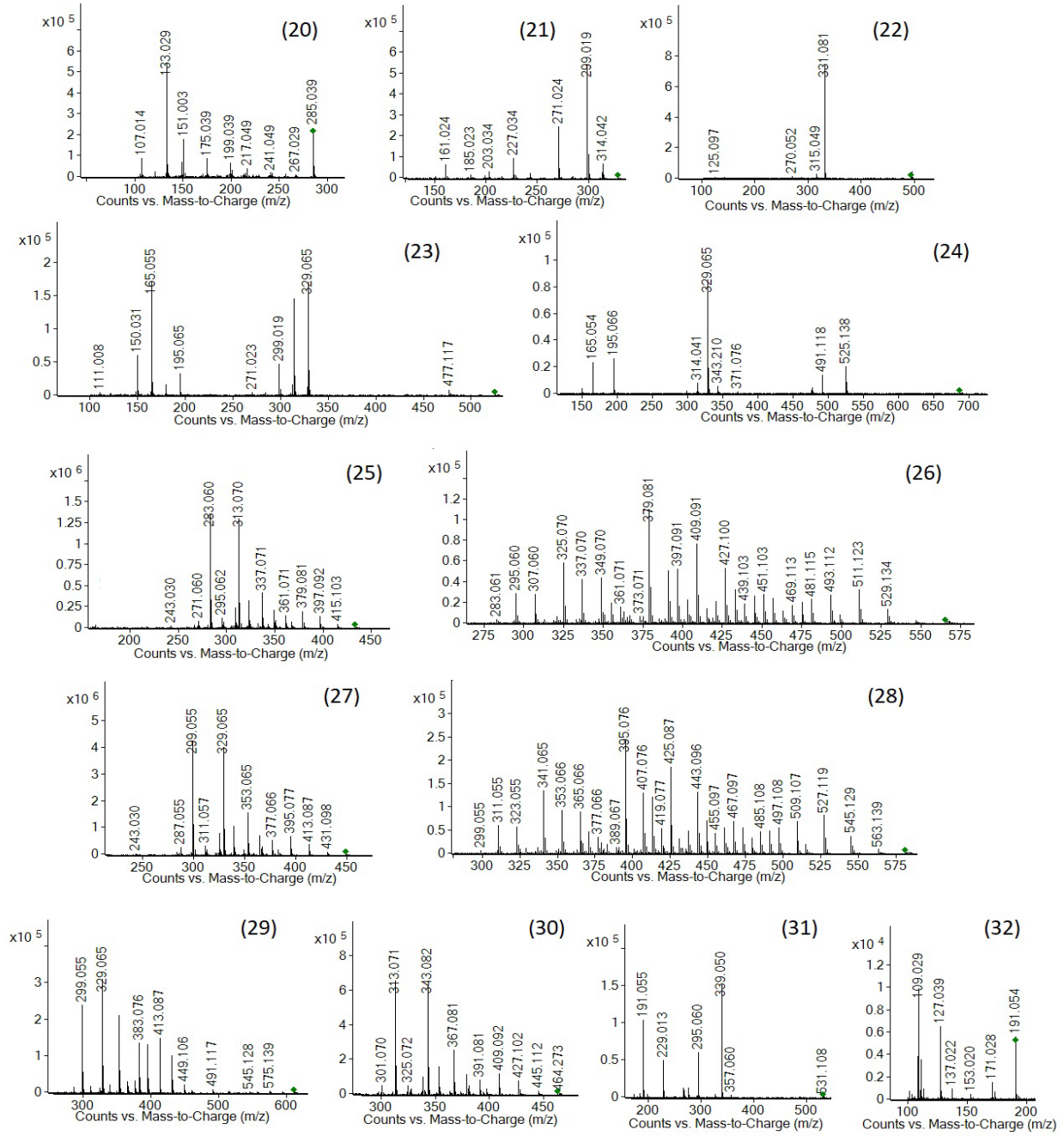


Figure S2. Fragmentation patterns (MS/MS spectra) of identified flavonoids and derivatives, and quinic acid: (**20**) Luteolin; (**21**) Tricin; (**22**) Tricin 7-*O*-hexoside or Tricin 5-*O*-hexoside*; (**23**) Tricin 4′-*O*-(erythro-β-guaiacyl-glyceryl)ether; (**24**) Tricin 4′-*O*-(erythro-β-guaiacyl-glyceryl) ether-7-*O*-hexoside; (**25**) Isovitexin (Apigenin-6-C-glucoside)*; (**26**) Isoschaftoside or Schaftoside (Apigenin-6,8-C-pentoside hexoside)*; (**27**) Isoorientin (Luteolin-6-C-glucoside)*; (**28**) Isocarlinoside or Carlinoside (Luteolin-6,8-C-pentoside hexoside)*; (**29**) Isoorientin 4'-O-glucoside*; (**30**) Isoscoparin (Chrysoeriol-6-C-glucoside)*; (**31**) Acacetin-6-C-(6"-O-malonyl)glucoside; (**32**) Quinic acid. *Compounds (MS/MS spectra) recorded in positive ionization mode.

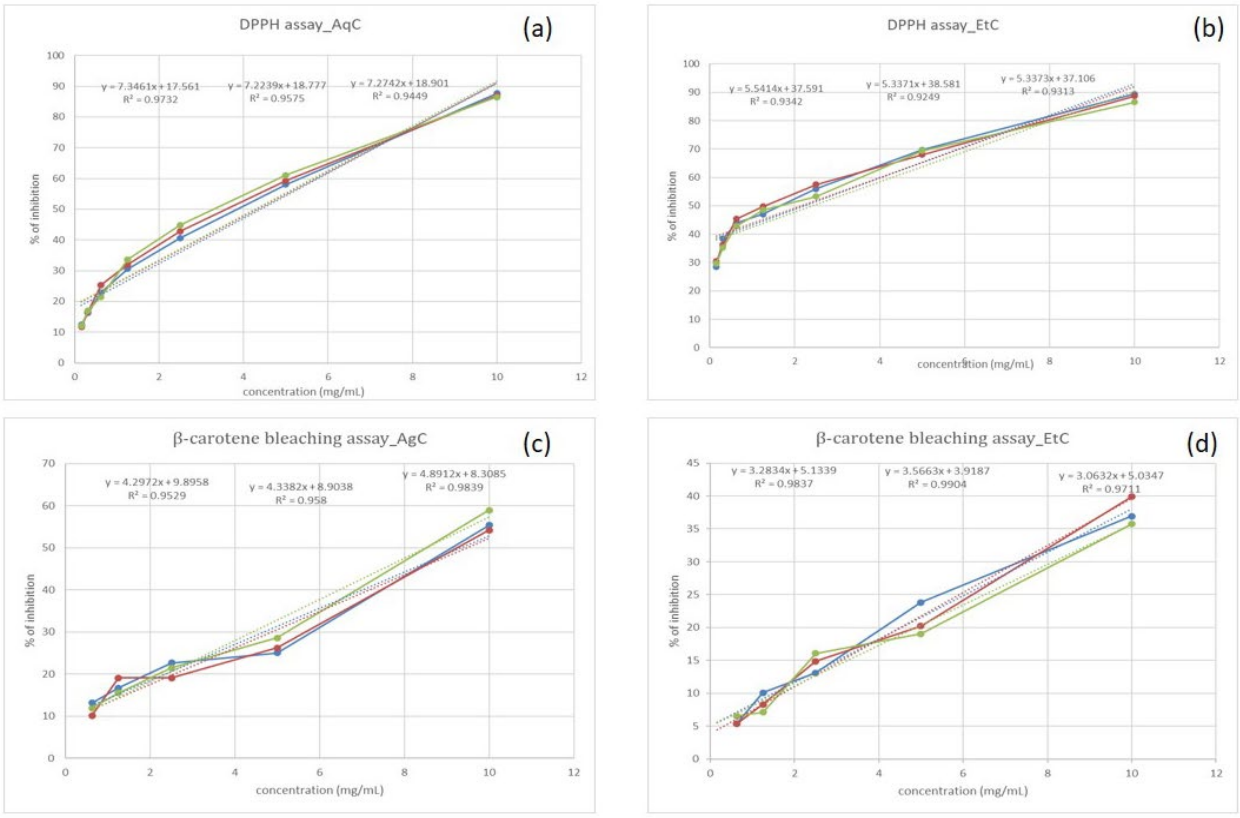


Figure S3. The DPPH (**a**,**b**) and β-caroten bleaching activity (**c**,**d**) of the control extracts at different concentrations (**a**,**c**—AqC, **b**,**d**—EtC). Note: The *x*-axis shows the concentration of sample (mg/mL) and the *y*-axis shows the percentage value of inhibition (%).

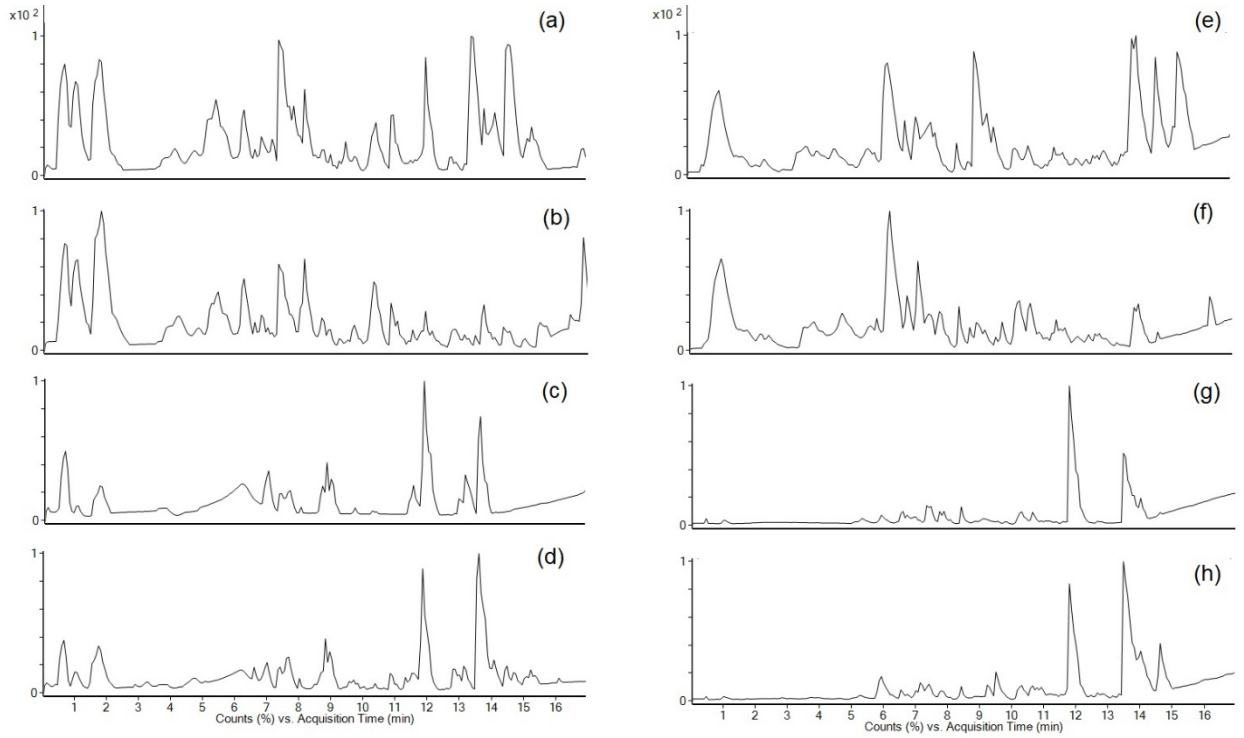


Figure S4. MS-Base peak chromatograms of: (**a**,**e**) Undigested (control) ethanolic extract (EtC); (**b**,**f**) Undigested (control) aqueous extract (AqC); (**c**,**g**) Crude digested aqueous extract (AqD); (**d**,**h**) Crude digested ethanolic extract (EtD); in positive ionisation mode (**a**–**d**) and negative ionisation mode (**e**–**h**); for peak annotation see retention time in Table 2.

Table S1. Emax with 95% CI for the highest tested concentration of extracts that produced measurable activity on colorectal cancer cells, and apropriate CI for these extracts.

Extracts	Cell line	Emax with 95% CI	SI
EtC (24 h)	HCT-116	88.41 (84.22-92.60)	1.16
	HaCat	103.13 (96.368-109.89)	
AqC (24 h)	HCT-116	76.72 (71.92-81.52)	1.39
	HaCat	106.87 (99.46-114.28)	
AqC (72 h)	HCT-116	81.61 (76.98-86.23)	1.30
	HaCat	106.41 (104.43-108.39)	
AqD (24 h)	HCT-116	83.53 (76.19-90.86)	1.35
	HaCat	113.33 (103.26-123.40)	