

Exploring the potential of the phenolic compounds from the coffee pulp in preventing cellular oxidative stress after *in vitro* digestion

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Supplementary Table 1. Correlation coefficients between phenolic compounds and methylxanthines, and the radical scavenging, cytoprotective properties, and cellular antioxidant activity in the coffee pulp flour (CPF) and extract (CPE).

Compounds	TPC	ABTS	FRAP	O ₂ ^{•-}	H ₂ O ₂	NO	ONOO ⁻	V IEC6	V HepG2	ROS IEC-6	ROS HepG2
Coffee pulp flour											
<i>Hydroxybenzoic acids</i>											
Gallic acid											
Gallic acid	-0.990**	-0.968*	-0.848	-0.930*	-0.532	-0.958*	-0.847	-0.750	-0.878	-0.772	-0.984**
Protocatechuic acid	0.366	0.448	0.506	0.217	0.839	0.167	-0.313	0.637	0.638	0.579	0.260
<i>Total</i>	0.046	0.138	0.237	-0.086	0.684	-0.147	-0.603	0.404	0.363	0.337	-0.060
<i>Hydroxycinnamic acids</i>											
3-Caffeoylquinic acid, 3-CQA											
3-Caffeoylquinic acid, 3-CQA	0.968*	0.978*	0.892	0.869	0.757	0.871	0.584	0.860	0.974*	0.856	0.926*
4-Caffeoylquinic acid, 4-CQA (<i>cis</i>)	0.972*	0.977*	0.914*	0.855	0.609	0.897	0.831	0.826	0.905*	0.851	0.941*
4-Caffeoylquinic acid, 4-CQA (<i>trans</i>)	-0.296	-0.194	-0.043	-0.416	0.470	-0.475	-0.832	0.144	0.046	0.077	-0.398
5-Caffeoylquinic acid, 5-CQA	0.947	0.861	0.605	0.991*	0.582	0.998*	0.999*	0.574	0.800	0.550	0.992*
3,5-Dicaffeoylquinic acid, 3,5-diCQA	0.621	0.674	0.661	0.500	0.862	0.457	-0.028	0.745	0.808	0.698	0.537
5-p-Coumaroylquinic acid, 5-CoQA	0.545	0.580	0.535	0.472	0.772	0.413	-0.117	0.625	0.716	0.572	0.479
<i>Total</i>	0.153	0.265	0.396	-0.033	0.802	-0.076	-0.495	0.556	0.489	0.495	0.028
<i>Flavones</i>											
Apigenin-6,8-di-C-glucoside											
Apigenin-6,8-di-C-glucoside	-0.072	0.104	0.413	-0.396	0.728	-0.372	-0.428	0.557	0.315	0.529	-0.240
<i>Flavonols</i>											
Quercetin-3,7-di- <i>O</i> -glucoside											
Quercetin-3,7-di- <i>O</i> -glucoside	0.513	0.677	0.905	0.080	0.917	0.150	0.240	0.920	0.754	0.931	0.327
Quercetin-3- <i>O</i> -rutinoside	0.283	0.473	0.771	-0.171	0.789	-0.100	-0.009	0.794	0.567	0.812	0.082
Quercetin-3- <i>O</i> -glucoside	0.283	0.410	0.566	0.047	0.906*	0.024	-0.340	0.710	0.622	0.659	0.143
<i>Total</i>	-0.356	-0.238	-0.045	-0.510	0.465	-0.556	-0.846	0.145	0.006	0.083	-0.471
<i>Methylxanthines</i>											
Caffeine											
Caffeine	0.921*	0.973*	0.974*	0.739	0.864	0.760	0.544	0.960*	0.999**	0.959*	0.843

Coffee pulp extract

Hydroxybenzoic acids

Gallic acid	-0.686	-0.443	0.686	0.449	0.096	-0.479	0.934*	-0.404	-0.864	0.682	0.583
Protocatechuic acid	-0.924*	-0.988**	0.956*	0.880	-0.765	-0.104	0.613	-0.509	-0.079	0.986**	0.973*
Total	-0.941*	-0.905*	0.966*	0.825	-0.547	-0.247	0.792	-0.527	-0.362	0.987**	0.943*

Hydroxycinnamic acids

3-Caffeoylquinic acid, 3-CQA	-0.743	-0.955	0.813	0.651	-0.962	-0.844	0.962	-0.083	-0.493	0.904	0.995*
4-Caffeoylquinic acid, 4-CQA (<i>cis</i>)	-0.645	-0.267	0.556	0.738	0.304	0.563	0.242	-0.993*	-0.854	0.399	0.064
4-Caffeoylquinic acid, 4-CQA (<i>trans</i>)	-0.880	-0.959*	0.888	0.956*	-0.888	0.302	0.251	-0.669	0.200	0.876	0.808
3,5-Dicaffeoylquinic acid, 3,5-diCQA	-0.771	-0.434	0.695	0.846	0.130	0.407	0.410	-0.998*	-0.933	0.555	0.240
Total	-0.576	-0.378	0.593	0.311	0.146	-0.645	0.976*	-0.215	-0.859	0.618	0.577

Flavones

Apigenin-6,8-di-C-glucoside	-0.840	-0.987*	0.884	0.827	-0.860	-0.099	0.513	-0.391	0.100	0.934	0.969*
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Flavonols

Quercetin-3- <i>O</i> -rutinoside	-0.862	-0.993**	0.903*	0.849	-0.851	-0.078	0.519	-0.429	0.075	0.946*	0.968*
Quercetin-3- <i>O</i> -glucoside	-0.888	-0.997**	0.924*	0.874	-0.839	-0.053	0.526	-0.475	0.046	0.959*	0.964*
Total	-0.871	-0.994**	0.910*	0.858	-0.847	-0.070	0.521	-0.444	0.066	0.951*	0.935*

Methylxanthines

Caffeine	-0.871	-0.997**	0.907*	0.877	-0.873	-0.005	0.468	-0.474	0.110	0.940*	0.947*
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TPC: Total Phenolic Content; ABTS: ABTS antioxidant capacity; FRAP: FRAP antioxidant capacity; $\text{O}_2^{\cdot -}$: $\text{O}_2^{\cdot -}$ scavenging; H_2O_2 : H_2O_2 scavenging; NO: NO scavenging; ONOO^- : ONOO^- scavenging; V-IEC-6: t-BHP-viability in IEC-6 cells; V-HepG2: t-BHP-viability in HepG2 cells; ROS IEC-6: ROS production in IEC-6 cells; ROS HepG2: ROS production in HepG2 cells.