

# **Radical Scavenging and Cellular Antioxidant Activity of the Cocoa Shell Phenolic Compounds after Simulated Digestion**

Silvia Cañas<sup>1,2</sup>, Miguel Rebollo-Hernanz<sup>1,2</sup>, Patricia Bermúdez-Gómez<sup>1,2</sup>, Pilar Rodríguez-Rodríguez,<sup>3</sup> Cheyenne Braojos<sup>1,2</sup>, Alicia Gil-Ramirez<sup>1,2</sup>, Vanesa Benítez<sup>1,2</sup>, Yolanda Aguilera<sup>1,2</sup>, María A. Martín-Cabrejas<sup>1,2\*</sup>

<sup>1</sup> Department of Agricultural Chemistry and Food Science, Faculty of Science, C/ Francisco Tomás y Valiente, 7. Universidad Autónoma de Madrid, 28049, Madrid, Spain.

<sup>2</sup> Institute of Food Science Research (CIAL, UAM-CSIC). C/ Nicolás Cabrera, 9. Universidad Autónoma de Madrid, 28049, Madrid, Spain.

<sup>3</sup> Department of Physiology, Faculty of Medicine, Universidad Autónoma de Madrid, C/Arzobispo Morcillo 2, 28029 Madrid, Spain

\* Correspondence: [maria.martin@uam.es](mailto:maria.martin@uam.es)

**Supplementary Table S1.** Correlation coefficients between phenolic compounds and methylxanthines, and the radical scavenging, cellular antioxidant activity, and cytoprotective properties of the cocoa shell flour (CSF) and extract (CSE).

Compounds	TPC	ABTS	FRAP	O <sub>2</sub> <sup>•−</sup>	H <sub>2</sub> O <sub>2</sub>	NO	ONOO <sup>−</sup>	V-IEC-6	V-HepG2	ROS IEC-6	ROS HepG2
<b>Cocoa shell flour</b>											
<i>Hydroxybenzoic acids</i>											
Gallic acid	0.811	0.963*	0.725	0.262	0.832	−0.414	0.985**	0.689	0.682	0.965*	0.384
Protocatechuic acid	0.433	0.738	0.559	−0.202	0.478	−0.645	0.925*	0.405	0.631	0.700	0.074
<i>Total</i>	0.674	0.899	0.681	0.064	0.706	−0.535	0.994**	0.591	0.687	0.883	0.264
<i>N-phenylpropenoyl-L-amino acids</i>											
<i>N</i> -Coumaroyl-L-aspartate <i>cis</i>	0.581	0.238	0.373	0.580	0.543	0.249	−0.173	0.573	0.194	0.198	0.757
<i>N</i> -Coumaroyl-L-aspartate <i>trans</i>	0.358	0.008	0.292	0.316	0.327	0.152	−0.414	0.462	0.161	−0.094	0.730
<i>N</i> -Coumaroyl-L-tyrosine	0.979*	0.984**	0.884	0.372	0.988**	−0.388	0.818	0.915*	0.788	0.930*	0.725
<i>N</i> -Caffeoyl-L-DOPA <i>cis</i>	−0.393	−0.056	−0.359	−0.271	−0.366	−0.075	0.371	−0.517	−0.236	0.065	−0.776
<i>Total</i>	0.687	0.391	0.592	0.418	0.664	−0.018	−0.033	0.749	0.442	0.285	0.903*
<i>Flavan-3-ols</i>											
(+)-Catechin	0.341	0.663	0.554	−0.359	0.393	−0.742	0.856	0.373	0.657	0.589	0.066
(−)-Epicatechin	−0.195	−0.485	−0.064	−0.132	−0.214	0.105	−0.799	0.030	−0.093	−0.624	0.387
<i>Total</i>	0.342	0.651	0.616	−0.447	0.398	−0.830	0.809	0.428	0.731	0.537	0.151
<i>Flavonols</i>											
Quercetin 3- <i>O</i> -glucoside	−0.979*	−0.984**	−0.884	−0.372	−0.988**	0.388	−0.818	−0.915*	−0.788	−0.930*	−0.725
Quercetin 3- <i>O</i> -arabinoside	−0.979*	−0.984**	−0.884	−0.372	−0.988**	0.388	−0.818	−0.915*	−0.788	−0.930*	−0.725
<i>Total</i>	−0.979*	−0.984**	−0.884	−0.372	−0.988**	0.388	−0.818	−0.915*	−0.788	−0.930*	−0.725
<i>Methylxanthines</i>											
Theobromine	0.765	0.892	0.955*	−0.152	0.804	−0.801	0.798	0.868	0.971*	0.727	0.679
Caffeine	0.777	0.871	0.979*	−0.155	0.815	−0.804	0.735	0.905*	0.989**	0.688	0.745
<i>Total</i>	0.769	0.888	0.961*	−0.153	0.808	−0.803	0.785	0.770	0.976*	0.719	0.696
<b>Cocoa shell extract</b>											

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<i>Hydroxybenzoic acids</i>											
Gallic acid	0.013	0.138	−0.270	0.369	0.606	−0.514	0.548	−0.302	−0.408	−0.259	−0.915*
Protocatechuic acid	−0.393	−0.194	0.405	0.969*	−0.250	0.210	−0.323	−0.014	−0.591	−0.405	−0.244
Total	−0.087	0.067	−0.125	0.549	0.444	−0.377	0.377	−0.256	−0.488	−0.317	−0.825
<i>N-phenylpropenoyl-L-amino acids</i>											
N-Coumaroyl-L-aspartate <i>cis</i>	−0.963*	−0.997**	0.899	0.277	−0.643	0.855	−0.105	−0.732	0.690	0.799	0.130
N-Coumaroyl-L-aspartate <i>trans</i>	−0.317	−0.331	−0.060	−0.084	0.535	−0.250	0.869	−0.850	0.380	0.500	−0.889
N-Coumaroyl-L-tyrosine	−0.810	−0.851	0.923*	0.257	−0.899	0.982**	−0.501	−0.343	0.567	0.609	0.576
N-Caffeoyl-L-aspartate	−0.997**	−0.991**	0.925*	0.445	−0.635	0.838	−0.128	−0.726	0.552	0.696	0.042
N-Caffeoyl-L-DOPA <i>cis</i>	−0.783	−0.863	0.849	0.071	−0.795	0.921*	−0.339	−0.448	0.727	0.750	0.517
N-Caffeoyl-L-DOPA <i>trans</i>	−0.989**	−0.998**	0.919*	0.385	−0.641	0.848	−0.120	−0.731	0.605	0.737	0.075
Total	−0.988**	−0.998**	0.895	0.367	−0.592	0.813	−0.060	−0.772	0.620	0.756	0.016
<i>Flavan-3-ols</i>											
(+)-Catechin	0.364	0.245	−0.650	−0.765	0.839	−0.668	0.940*	−0.390	0.393	0.333	−0.623
(−)-Epicatechin	0.512	0.431	−0.786	−0.678	0.947*	−0.826	0.922*	−0.239	0.154	0.100	−0.698
Total	0.406	0.295	−0.690	−0.749	0.872	−0.713	0.940*	−0.351	0.333	0.274	−0.645
<i>Flavonols</i>											
Quercetin 3- <i>O</i> -glucoside	−0.987**	−0.998***	0.918*	0.376	−0.641	0.849	−0.119	−0.732	0.613	0.743	0.080
Quercetin 3- <i>O</i> -arabinoside	−0.977*	−0.999***	0.910*	0.327	−0.643	0.853	−0.112	−0.733	0.652	0.772	0.105
Total	−0.977*	−0.999***	0.910*	0.327	−0.643	0.853	−0.112	−0.733	0.652	0.772	0.105
<i>Flavones</i>											
Apigenin-6,8-di- <i>C</i> -glucoside	−0.786	−0.812	0.932*	0.323	−0.941*	0.993**	−0.589	−0.257	0.478	0.520	0.626
<i>Methylxanthines</i>											
Theobromine	−0.667	−0.616	0.363	0.369	0.133	0.133	0.520	−0.872	0.279	0.471	−0.735
Caffeine	−0.785	−0.759	0.503	0.331	−0.018	0.302	0.450	−0.933*	0.439	0.621	−0.600
Total	−0.668	−0.617	0.364	0.368	0.132	0.134	0.520	−0.873	0.280	0.472	−0.734

TPC: Total Phenolic Content; ABTS: ABTS antioxidant capacity; FRAP: FRAP antioxidant capacity; O<sup>2•−</sup>: O<sup>2•−</sup> scavenging; H<sub>2</sub>O<sub>2</sub>: H<sub>2</sub>O<sub>2</sub> scavenging; NO: NO scavenging; ONOO<sup>−</sup>: ONOO<sup>−</sup> scavenging; V-IEC-6: viability-IEC-6; V-HepG2: viability-HepG2; ROS IEC-6: reactive oxygen species IEC-6; ROS HepG2: reactive oxygen species HepG2.