

LCBS

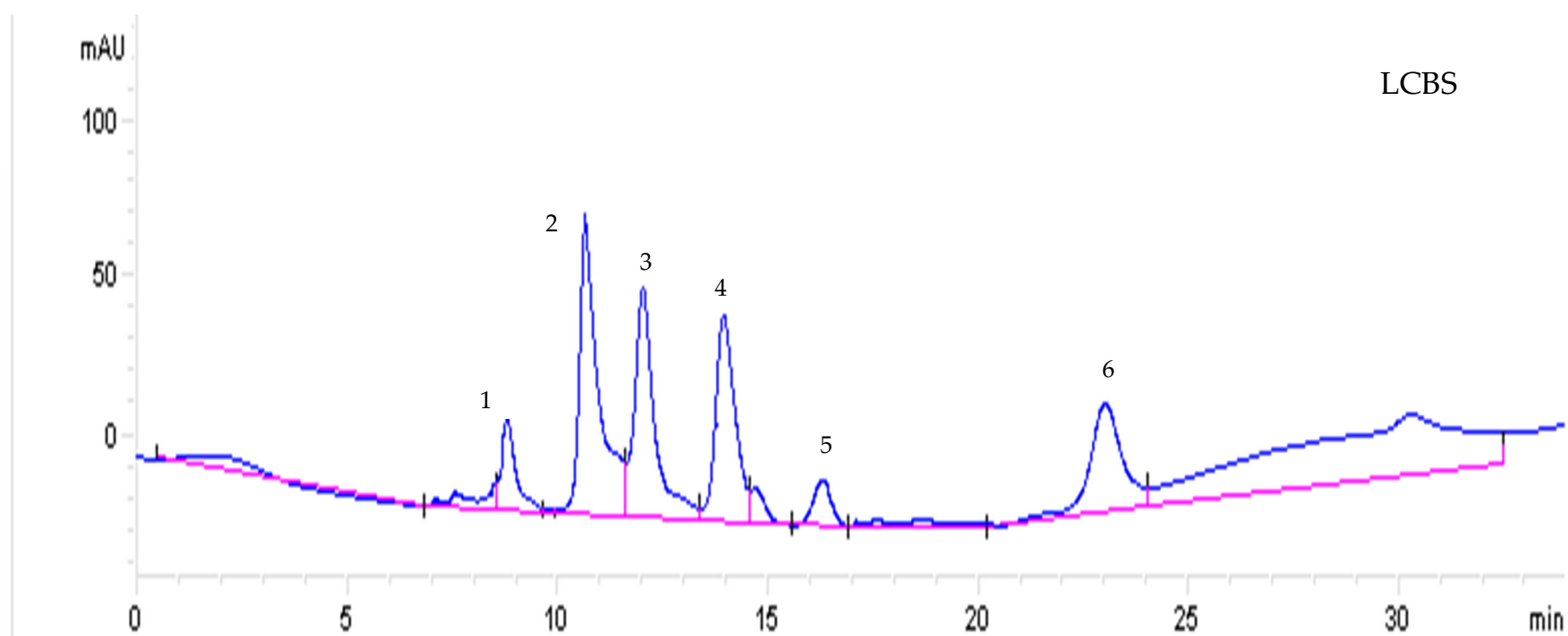


Figure S1. Chromatographic profile of organic acids found in LCBS samples. 1: Oxalic acid; 2: citric acid, 3: Succinic acid, 4: Tartaric acid, 5: Malic acid, 6: Acetic acid

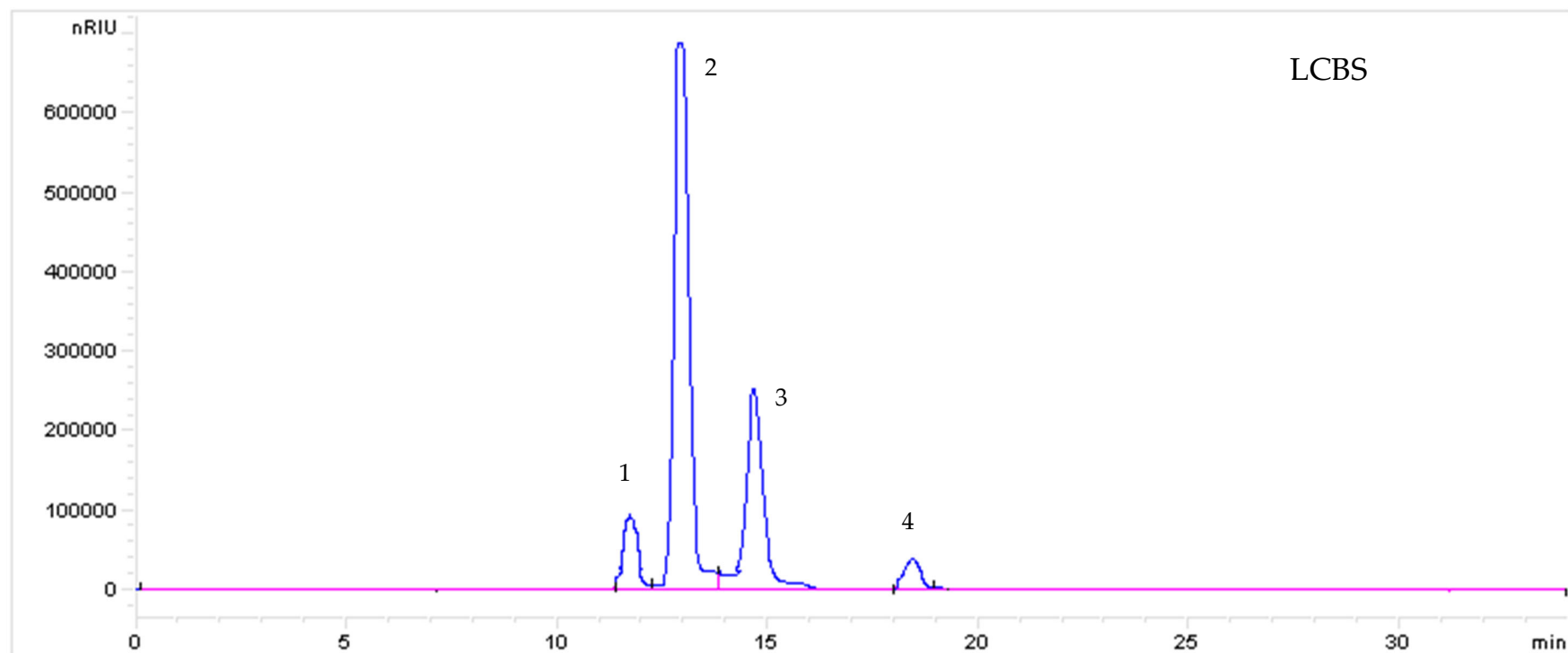


Figure S2. Chromatographic profile of sugars found in LCBS samples. 1: sucrose; 2: glucose, 3: fructose, 4: Arabinose

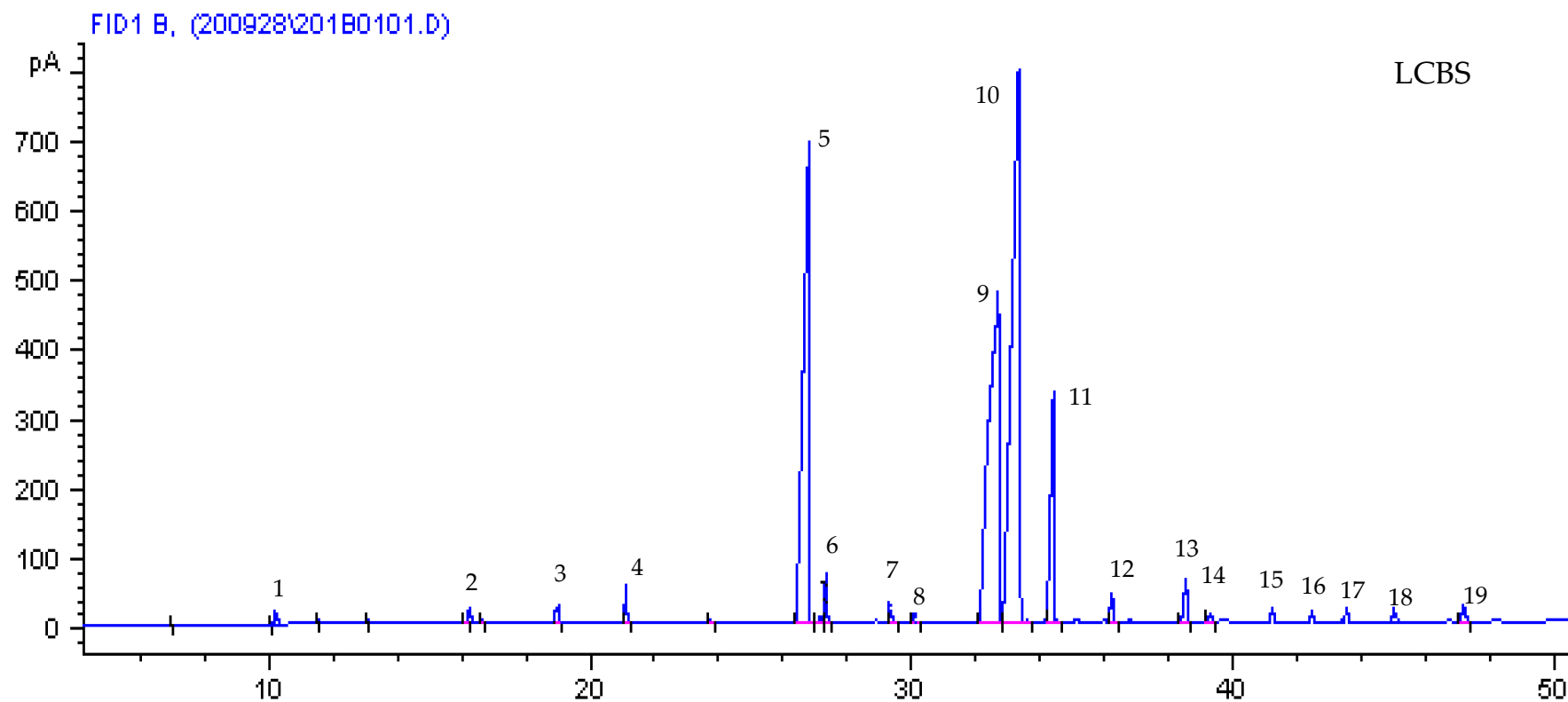
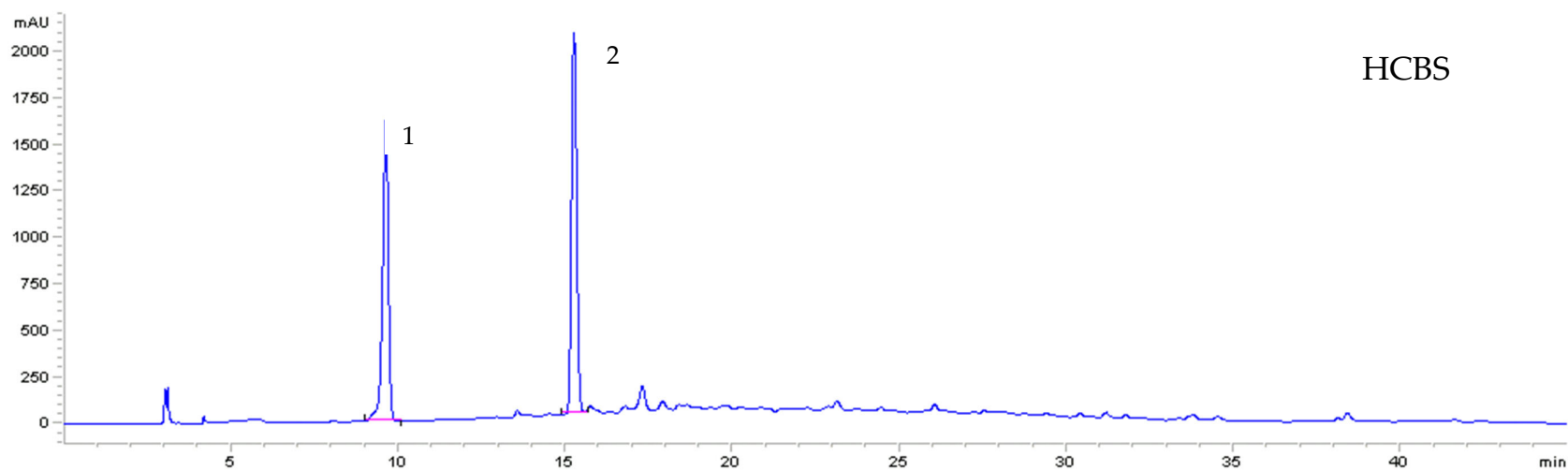
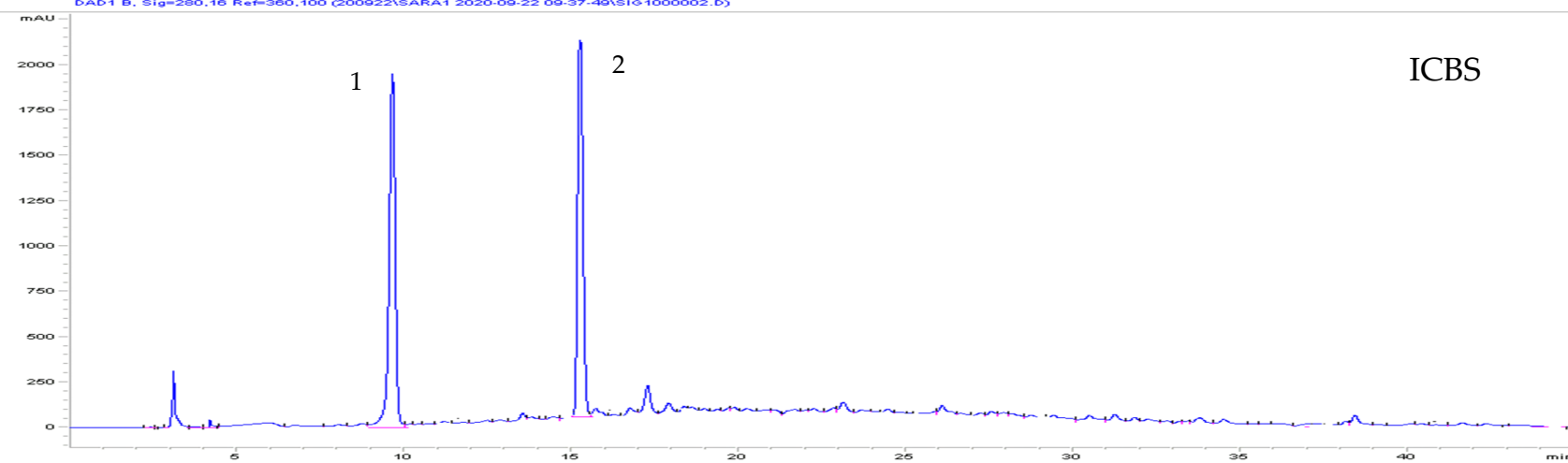


Figure S3. Chromatographic profile of fatty acids found in LCBS samples. 1: C10:0; 2: C12:0; 3: C14:0; 4: C15:0; 5: C16:0; 6: C16:1; 7: C17:0; 8: C17:1; 9: C18:0; 10: C18:1; 11: C18:2; 12: C18:3; 13: C20:0; 14: C20:1; 15: C20:2; 16: C20:3; 17: C22:0; 18: C22:5; 19: C24:0



DAD1 B, Sig=280,16 Ref=360,100 (200922\SARA1 2020-09-22 09-37-49\SIG-1000002.D)



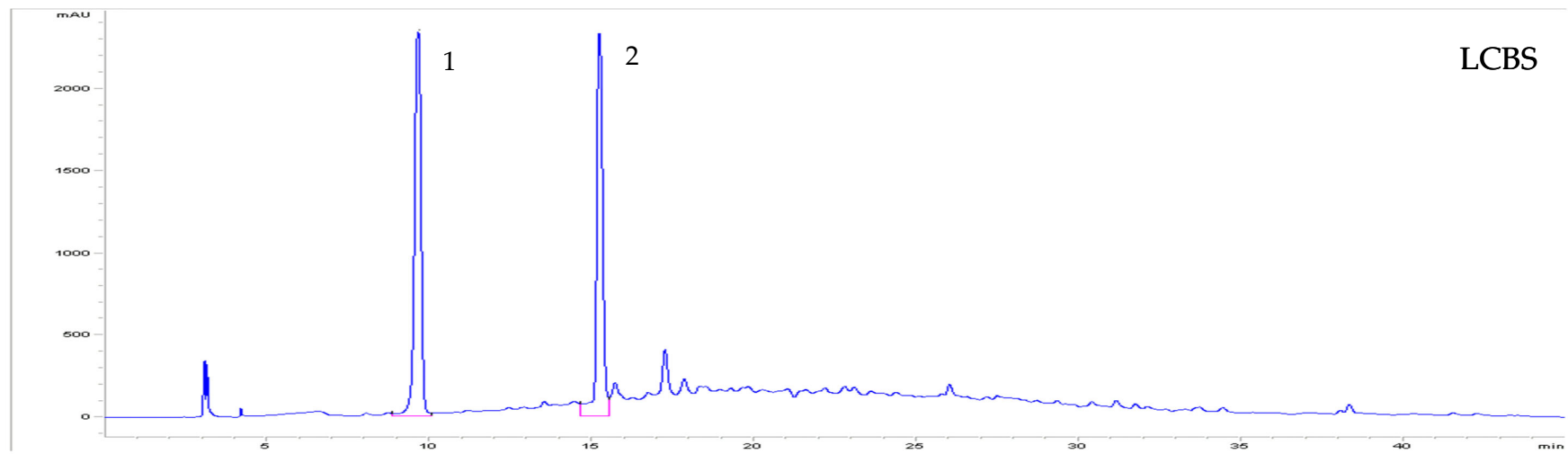


Figure S4. Chromatographic profile of methylxanthines found in HCBS, ICBS and LCBS samples. 1: Theobromine; 2: caffeine

Table S1. Pearson's correlation coefficients between the different antioxidant assays (DPPH, ABTS, FRAP and FIC) and the main bioactive compounds founds in LCBS samples.

	<i>Theobromine</i>	<i>Caffeine</i>	<i>Epicatechin</i>	<i>Epicatechin derivative</i>	<i>Catechin</i>	<i>Quercetin</i>	<i>Protocatechuic acid</i>	<i>DPPH</i>	<i>ABTS</i>	<i>FRAP</i>	<i>FIC</i>
Theobromine	1.00										
Caffeine	1.00	1.00									
Epicatechin	0.960	0.960	1.00								
Epicatechin derivative	-0.419	-0.419	-0.657	1.00							
Catechin	0.771	0.771	0.561	0.255	1.00						
Quercetin	0.182	0.182	-0.101	0.816	0.767	1.00					
Protocatechuic acid	-0.608	-0.608	-0.807	0.976	0.036	0.669	1.00				
DPPH	0.500	0.500	0.723	-0.996	-0.166	-0.760	-0.991	1.00			
ABTS	0.264	0.264	0.824	-0.986	-0.411	-0.900	-0.926	0.967	1.000		
FRAP	-0.277	-0.277	-0.536	0.989	0.398	0.894	0.931	-0.971	-1.000	1.000	
FIC	0.998	0.998	0.976	-0.476	0.729	0.119	-0.658	0.554	0.325	-0.338	1.000

Table S2. Pearson's correlation coefficients between the different antioxidant assays (DPPH, ABTS, FRAP and FIC) and the main bioactive compounds founds in ICBS samples.

	<i>Theobromine</i>	<i>Caffeine</i>	<i>Epicatechin</i>	<i>Epicatechin derivative</i>	<i>Catechin</i>	<i>Quercetin</i>	<i>Protocatechuic acid</i>	<i>DPPH</i>	<i>ABTS</i>	<i>FRAP</i>	<i>FIC</i>
Theobromine	1.000										
Caffeine	0.982	1.000									
Epicatechin	0.619	0.459	1.000								
Epicatechin derivative	0.673	0.801	-0.164	1.000							
Catechin	-0.346	-0.517	0.523	-0.926	1.000						
Quercetin	0.788	0.658	0.971	0.076	0.305	1.000					
Protocatechuic acid	0.672	0.520	0.998	-0.095	0.462	0.985	1.000				
DPPH	0.397	0.317	0.967	-0.411	0.724	0.878	0.946	1.000			
ABTS	-0.554	-0.387	0.997	0.242	-0.589	-0.949	-0.989	-0.984	1.000		
FRAP	0.961	0.891	0.812	0.442	-0.072	0.928	0.851	0.636	-0.763	1.000	
FIC	0.500	0.655	-0.371	0.977	-0.985	-0.139	-0.305	-0.596	0.444	0.240	1

Table S3. Pearson's correlation coefficients between the different antioxidant assays (DPPH, ABTS, FRAP and FIC) and the main bioactive compounds founds in HCBS samples.

	<i>Theobromine</i>	<i>Caffeine</i>	<i>Epicatechin</i>	<i>Epicatechin derivative</i>	<i>Catechin</i>	<i>Quercetin</i>	<i>Protocatechuic acid</i>	<i>DPPH</i>	<i>ABTS</i>	<i>FRAP</i>	<i>FIC</i>
Theobromine	1.00										
Caffeine	-0.380	1.00									
Epicatechin	1.000	-0.371	1.00								
Epicatechin derivative	0.957	-0.096	0.960	1.00							
Catechin	-1.000	0.379	-1.000	-0.958	1.00						
Quercetin	-0.549	0.982	-0.541	-0.285	0.548	1.00					
Protocatechuic acid	0.959	-0.101	0.961	1.000	-0.959	-0.289	1.00				
DPPH	0.444	0.661	0.452	0.684	-0.445	0.505	0.680	1.00			
ABTS	0.961	0.908	0.963	1.000	-0.961	-0.296	1.000	0.675	1.00		
FRAP	-0.655	-0.451	-0.662	-0.845	0.656	-0.272	-0.843	-0.968	-0.839	1.00	
FIC	0.952	0.998	-0.319	-0.041	-0.327	0.970	-0.046	0.701	-0.053	-0.499	1.00