

SUPPLEMENTARY MATERIAL

Black tea samples origin discrimination using analytical investigations of secondary metabolites, antiradical scavenging activity and chemometric approach

Wojciech Koch, Wirginia Kukula-Koch, Łukasz Komsta

Figure S1. Fragmentation patterns of the investigated catechins and gallic acid recorded in the negative ionization mode of LC-ESI-Q-TOF-MS spectrometry (the Y axis values for more clear view are divided by 10).

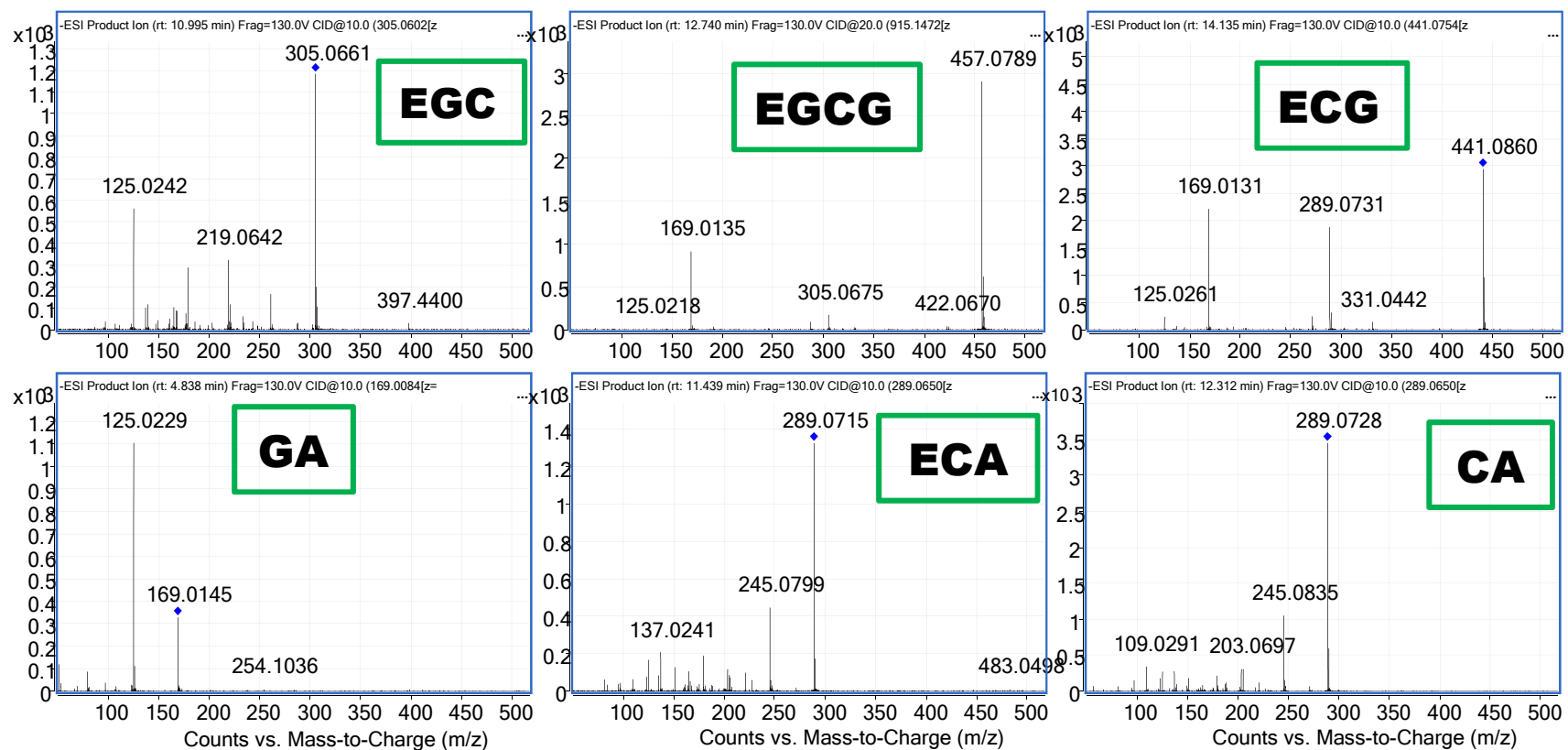


Figure S2. Statistical significance of each parameter, separately.

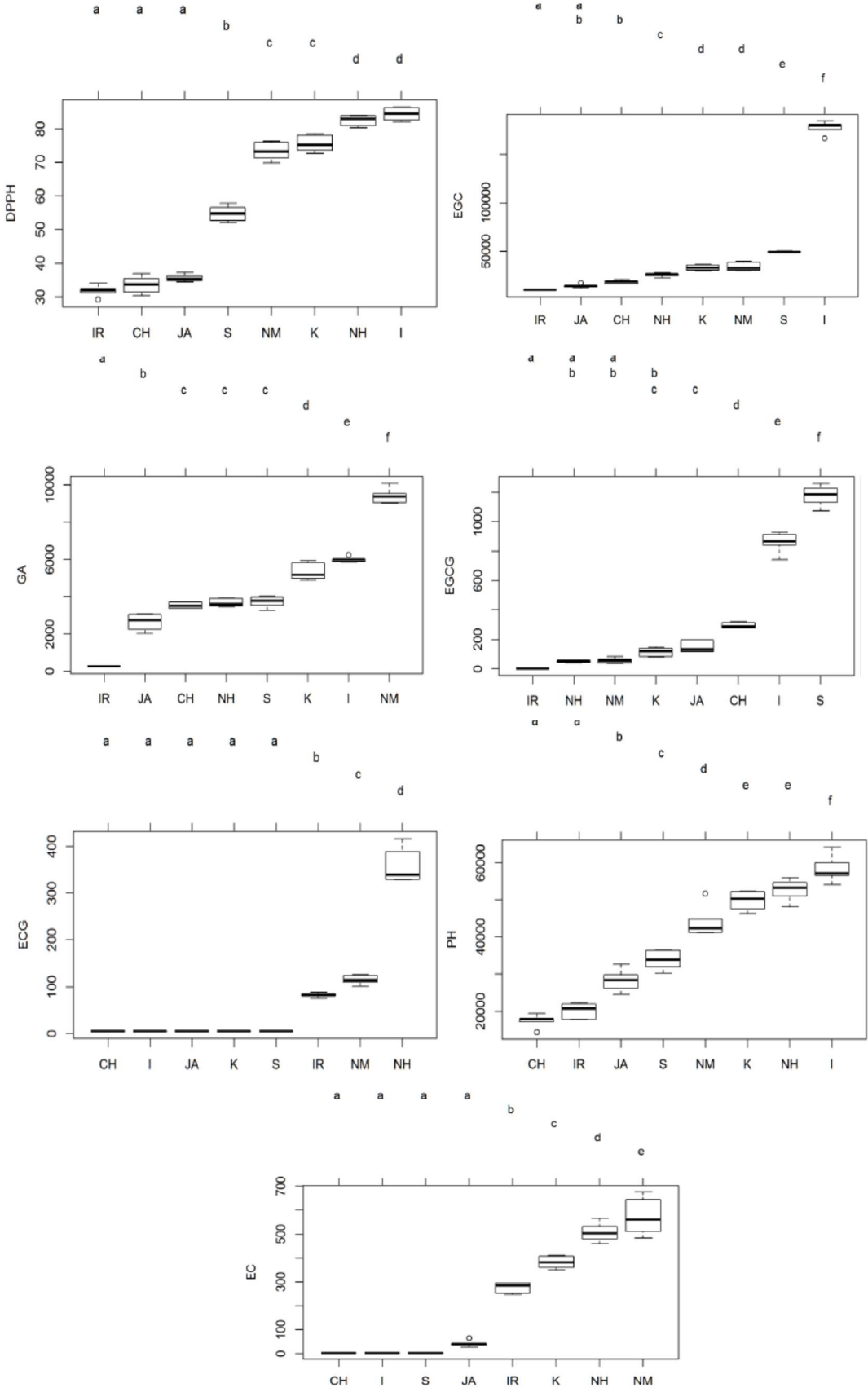


Table S1. Correlation of individual parameters in pairs and its significance.

	lower	r	upper	p
DPPH-GA	0.4716	0.6664	0.7992	2.334e-07
DPPH-EGC	0.3231	0.5562	0.7256	4.052e-05
DPPH-EGCG	-0.1464	0.1437	0.411	0.3299
DPPH-ECG	0.1233	0.3937	0.6096	0.005637
DPPH-EC	0.204	0.4614	0.6591	0.0009635
DPPH-PH	0.92	0.9546	0.9744	0
GA-EGC	0.0888	0.3638	0.5872	0.01104
GA-EGCG	-0.2137	0.07496	0.3516	0.6126
GA-ECG	-0.2788	0.005824	0.2895	0.9687
GA-EC	0.1149	0.3864	0.6042	0.00667
GA-PH	0.3686	0.5909	0.7492	9.802e-06
EGC-EGCG	0.3943	0.6101	0.7621	4.157e-06
EGC-ECG	-0.481	-0.228	0.05998	0.119
EGC-EC	-0.5667	-0.3368	-0.05828	0.01923
EGC-PH	0.3855	0.6035	0.7577	5.607e-06
EGCG-ECG	-0.6251	-0.4147	-0.148	0.003385
EGCG-EC	-0.7894	-0.6513	-0.4506	5.35e-07
EGCG-PH	-0.1401	0.15	0.4164	0.3087
ECG-EC	0.4796	0.6721	0.8029	1.684e-07
ECG-PH	0.05044	0.3298	0.5614	0.02205
EC-PH	0.1034	0.3765	0.5968	0.008348

Table S2. The raw data obtained from Principal Components Analysis.

Principal Components Analysis

	PC1	PC2	PC3	PC4	PC5	PC6	PC7		
DPPH	0.5504	-0.04181	0.1044	-0.001019	0.2546	-0.06312	0.7846		
GA	0.4204	-0.06352	-0.6959	-0.3386	-0.4034	-0.2212	-0.09303		
EGC	0.2985	-0.4795	0.1619	0.4605	-0.5027	0.432	-0.05806		
EGCG	0.03593	-0.5603	0.2326	-0.7094	0.2131	0.2521	-0.1358		
ECG	0.2375	0.4339	0.6101	-0.3221	-0.4986	-0.1582	-0.07601		
EC	0.3013	0.5057	-0.1662	-0.07693	0.2237	0.7341	-0.1759		
PH	0.5317	-0.07977	0.1572	0.2456	0.4192	-0.3647	-0.5632		
			PC1	PC2	PC3	PC4	PC5	PC6	PC7
Standard deviation			1.779	1.572	0.8626	0.5737	0.4149	0.3002	0.1679
Proportion of Variance			0.4521	0.3531	0.1063	0.04702	0.02459	0.01288	0.00403
Cumulative Proportion			0.4521	0.8052	0.9115	0.9585	0.9831	0.996	1

Table S3. The analysis of variance (ANOVA) for all parameters.

Parameter	F value	Pr(>F)
DPPH	731.7	3.969e-40
GA	489.9	1.112e-36
EGC	1936	1.566e-48
EGCG	732.6	3.876e-40
ECG	492.7	9.932e-37
EC	332.7	2.263e-33
PH	176.9	5.002e-28

Figure S3. Biplot figure.

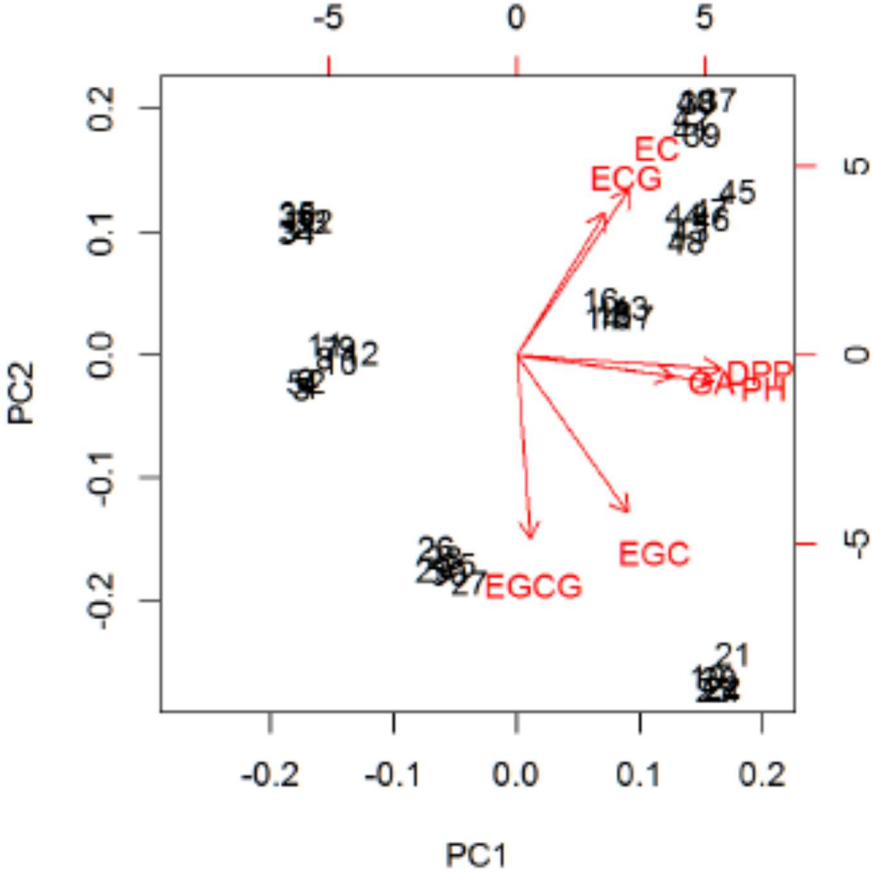


Table S4. The analysis of variance (ANOVA) for each parameter separately.

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
DPPH	7	21835	3119	731.7	3.969e-40
DPPH	40	170.5	4.263	NA	NA
GA	7	302171663	43167380	489.9	1.112e-36
GA	40	3524580	88115	NA	NA
EGC	7	1.275e+11	1.822e+10	1936	1.566e-48
EGC	40	376468542	9411714	NA	NA
EGCG	7	7977818	1139688	732.6	3.876e-40
EGCG	40	62230	1556	NA	NA
ECG	7	634588	90655	492.7	9.932e-37
ECG	40	7360	184	NA	NA
EC	7	2449540	349934	332.7	2.263e-33
EC	40	42075	1052	NA	NA
PH	7	9.891e+09	1.413e+09	176.9	5.002e-28
PH	40	319581667	7989542	NA	NA