SUPPLMENTARY MATERIAL

Green tea quality evaluation based on its catechins and metals composition in combination with chemometric analysis

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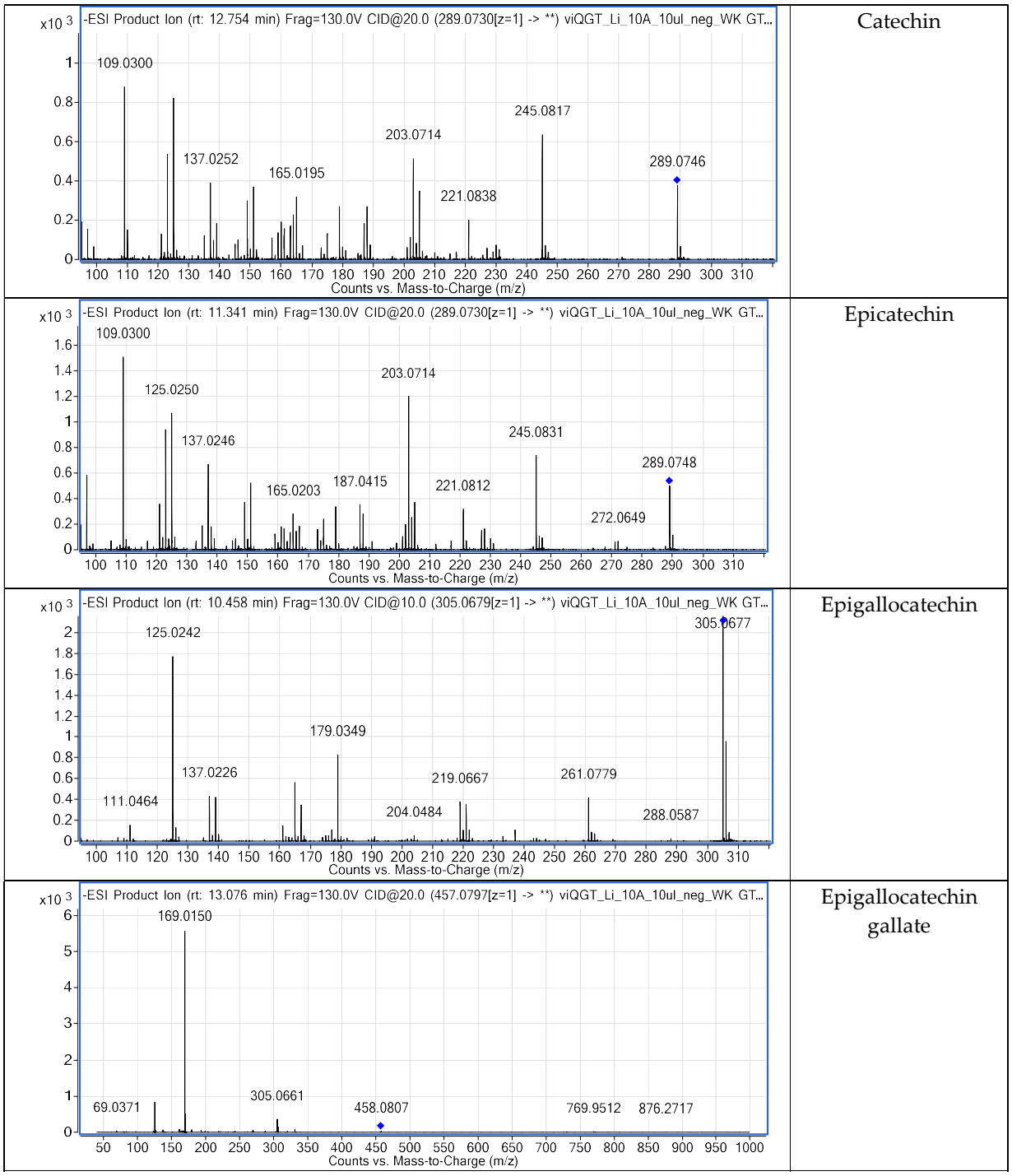
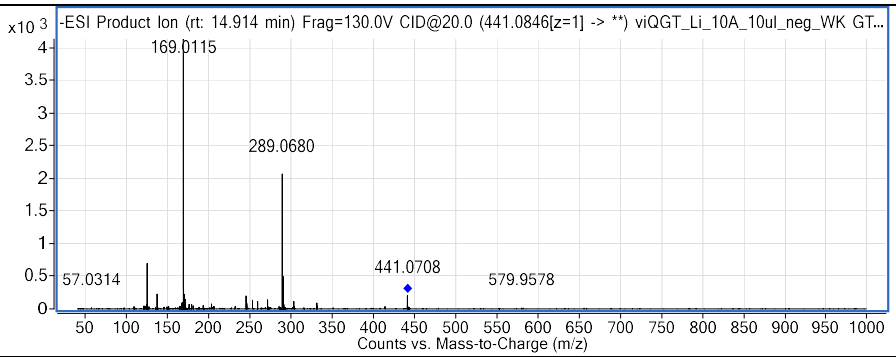
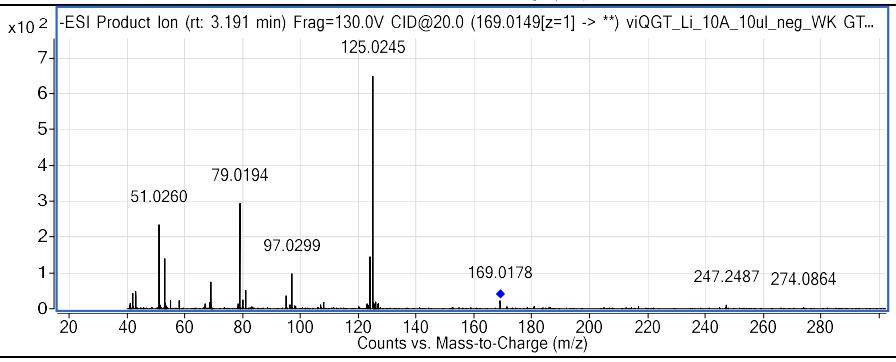
Table S1. Accurate mass measurements and identification data of catechins in the studied samples.

No	*Ion (+/-)*	*Rt (min)*	*Molecular formula*	*m/z experimental*	*m/z calculated*	*Delta (ppm)*	*DBE*	*MS/MS fragments*	*Proposed compound*
1	(-)	12.6	$C_{15}H_{14}O_6$	289.0717	289.0718	0.21	9.0	245, 203, 165	**Catechin**
2	(-)	11.4	$C_{15}H_{14}O_6$	289.0721	289.0718	-1.17	9.0	245, 203, 163	**Epicatechin**
3	(-)	10.2	$C_{15}H_{14}O_7$	305.0671	305.0667	-1.38	9.0	261, 219, 179, 167	**Epigallocatechin**
4	(-)	14.2	$C_{22}H_{18}O_{11}$	457.0790	457.0776	-2.98	14.0	305, 169	**Epigallocatechin gallate**
5	(-)	15.1	$C_{22}H_{18}O_{10}$	441.0841	441.0827	-3.12	14.0	289, 169	**Epicatechin gallate**
6	(-)	3.2	$C_9H_8O_4$	169.0150	169.0142	-4.43	5.0	125, 97	**Gallic acid**

Figure S1. Fragmentation spectra of all identified catechins and gallic acid obtained at the collision energy of 20V in the negative ionization mode.



	Epicatechin gallate
	Gallic acid

PCA Summary and Scores

Dataset S1. The raw data obtained from Principal Components Analysis.

Table continues below

	PC1	PC2	PC3	PC4	PC5
Standard deviation	2.662	2.22	1.566	1.346	1.168
Proportion of Variance	0.3374	0.2348	0.1167	0.08627	0.06498
Cumulative Proportion	0.3374	0.5722	0.6889	0.7752	0.8401

Table continues below

	PC6	PC7	PC8	PC9	PC10
Standard deviation	0.9327	0.8342	0.6271	0.6098	0.5015
Proportion of Variance	0.04142	0.03314	0.01873	0.01771	0.01198
Cumulative Proportion	0.8816	0.9147	0.9334	0.9511	0.9631

Table continues below

	PC11	PC12	PC13	PC14	PC15
Standard deviation	0.4155	0.3822	0.3613	0.268	0.2565
Proportion of Variance	0.00822	0.00696	0.00622	0.00342	0.00313

Cumulative Proportion	0.9713	0.9783	0.9845	0.9879	0.991

Table continues below

	PC16	PC17	PC18	PC19	PC20
Standard deviation	0.2399	0.211	0.1876	0.1622	0.1262
Proportion of Variance	0.00274	0.00212	0.00168	0.00125	0.00076
Cumulative Proportion	0.9938	0.9959	0.9976	0.9988	0.9996

	PC21
Standard deviation	0.09146
Proportion of Variance	4e-04
Cumulative Proportion	1

Table continues below

PC1	PC2	PC3	PC4	PC5	PC6	PC7
-1.208	3.567	-0.4406	2.068	2.159	0.8809	-0.005901
-1.426	3.481	0.1338	1.997	0.7142	2.46	0.4478
-1.454	3.473	0.2349	1.572	1.61	1.068	-0.423
-1.116	3.285	-0.7634	1.497	2.767	0.5978	-0.3718
-1.419	3.058	-0.1135	1.895	1.734	0.5771	-0.7232
-1.399	3.517	-0.7839	1.176	0.6647	1.292	-0.05869
-1.395	3.803	-0.4604	1.329	0.7515	1.074	-0.04702
-1.198	3.474	0.1575	1.453	2.509	0.5237	0.03556
-1.585	3.205	-0.4896	1.49	0.4394	1.87	-0.0455
4.961	-1.108	-1.503	0.7523	-0.2467	0.4477	0.6496
5.818	-0.2463	-1.157	1.018	0.5381	-0.8099	0.2163
4.816	-0.9127	-1.696	0.2342	0.2332	-0.4638	-0.1152
4.415	-0.2519	-0.8184	-0.1008	-0.1015	-0.3296	0.4588
5.126	-0.3736	-0.7052	0.7357	-0.01584	-1.024	-0.155
5.669	-0.6722	-1.135	0.9683	-0.1955	-0.2981	0.3957
5.089	-1.099	-1.416	0.882	0.006128	0.3551	0.04222
5.261	-0.334	-1.648	0.36	0.03929	-0.3362	0.6179
5.103	-0.3943	-0.9838	0.5279	0.001402	-0.3324	0.8439
4.036	0.06305	-0.7865	-0.3261	0.1085	0.06531	-0.08024
3.383	-0.182	-1.348	-0.08731	-0.3863	0.2882	-0.5469
4.149	0.3915	-0.3539	-0.483	0.2489	-0.7719	-0.5958
2.917	0.6833	-1.487	-1.187	-0.9864	1.174	-0.04531
3.615	0.3662	-1.364	-0.8602	-0.7114	0.3999	-0.3125
3.931	0.1429	-1.518	-0.8177	-0.6489	0.7844	0.2089
3.729	0.2901	-0.7839	-0.305	0.00723	-0.06093	-0.2312
4.211	0.1179	-0.6834	-0.2574	0.5185	-0.399	-0.01262
3.65	0.1876	-1.336	-0.3645	-0.1508	0.6011	-0.61
-0.7981	3.742	0.3759	0.2708	-0.1586	-1.027	-0.7379
-0.4644	3.646	0.89	-0.3103	-0.5916	-1.226	0.4747
-0.6029	3.58	1.317	-0.01376	-3.61	-0.5962	0.09034
-0.9018	3.375	1.569	0.35	-3.422	-0.3616	0.5507
-1.169	3.083	0.972	0.5147	-2.894	-0.3146	-0.2675
-0.7759	2.769	0.7461	-0.2029	-3.312	0.5706	-0.1031

-0.7349	3.994	0.6206	1.098	-1.694	-0.1683	-0.4787
-0.469	3.535	1.092	0.6531	-2.29	-0.459	-0.08084
-0.726	2.939	0.7558	-0.4746	-1.876	-1.634	-0.3121
-1.207	1.376	-0.0236	-2.089	1.926	0.1665	1.686
-1.728	1.23	0.09168	-2.068	1.046	-0.8748	0.9329
-1.805	1.95	-0.7711	-2.597	0.692	-0.7782	0.3566
-1.331	1.459	0.03994	-3.28	0.6333	-0.5535	1.371
-0.981	0.9928	-0.2932	-2.727	0.2625	-0.3084	0.9029
-1.528	1.292	-0.157	-2.448	1.483	-1.524	0.6542
-1.61	0.9778	-0.6302	-2.258	1.812	-1.326	0.1352
-1.742	2.208	0.2927	-2.077	0.1821	0.517	1.669
-1.533	1.582	0.1207	-2.651	1.163	-1.516	0.6348
-2.639	-2.304	0.1249	2.429	0.63	-1.639	1.015
-2.459	-2.809	-1.111	1.54	0.1797	-1.071	0.5001
-2.573	-2.672	-0.6589	1.889	-0.8579	-0.03674	1.632
-2.834	-3.226	-0.4423	1.85	-1.452	-0.2199	1.471
-2.926	-2.215	-0.1052	2.372	-0.02292	-0.8741	0.7179
-2.443	-2.245	-0.641	2.525	0.3634	-0.8641	1.159
-2.378	-2.667	-0.2378	1.622	-0.7938	-0.3073	1.535
-2.452	-2.529	-0.5951	1.885	0.03575	-1.049	1.233
-2.842	-2.998	-0.8999	2.381	0.0174	-1.06	0.2374
-1.7	-1.956	-0.6263	0.07483	-0.2251	-0.03504	-1.774
-1.555	-0.1897	-0.2766	-0.1955	0.8031	-1.589	-1.632
-1.94	-1.584	-0.7439	-0.07026	-0.7471	0.5417	-1.718
-1.939	-1.05	-0.6401	-0.5017	-0.02944	-0.5549	-1.273
-1.978	-1.045	-0.4493	0.1572	0.4665	-1.354	-1.942
-1.654	-1.363	-0.6936	-0.1993	0.4713	-0.7208	-1.505
-1.561	-1.46	-0.5613	-0.3783	-0.4091	0.1367	-1.349
-1.918	-1.247	-0.6493	0.1739	-0.2501	0.1167	-1.648
-2.08	-0.6508	-0.3124	-0.4138	-0.008613	-1.322	-1.644
1.449	-1.539	3.831	-0.03676	0.6951	-0.08344	-0.03675
1.585	-2.116	4.036	-0.2707	-0.1091	1.209	0.2986
1.873	-1.975	3.071	-0.3527	1.013	0.4391	-0.6476
0.8353	-1.349	3.88	0.4334	1.038	-1.13	-0.8257
1.034	-2.129	4.353	0.3913	0.4804	0.2776	-0.55
1.876	-1.79	4.544	-0.3872	0.2099	1.228	0.9685

1.502	-1.847	4.303	-0.4946	0.191	0.6695	0.4962
1.098	-1.139	3.764	-0.0181	0.8057	-0.2438	-0.6657
1.524	-2.512	3.55	-0.2523	0.3248	0.844	-0.3834
-2.395	-2.411	-1.55	-1.392	-0.582	1.313	-0.1739
-2.196	-2.713	-1.419	-0.7367	-0.2175	1.566	-0.3535
-2.244	-2.351	-0.9756	-1.207	-0.5542	1.105	-0.3362
-2.076	-2.256	-0.8126	-1.275	-0.3986	1.275	0.1479
-2.256	-2.077	-1.021	-1.268	-0.05443	1.031	0.2425
-2.187	-1.924	-0.5968	-1.15	-0.1849	0.6769	0.01097
-2.231	-2.532	-1.143	-1.29	-0.4351	0.9092	-0.5241
-2.747	-2.267	-1.223	-1.215	-0.7955	1.196	-0.2139
-2.15	-2.126	-0.8322	-1.475	-0.5571	1.401	0.5153

Table continues below

PC8	PC9	PC10	PC11	PC12	PC13	PC14
-0.07301	-0.4367	-0.2642	0.5096	-0.2555	0.2562	-0.1207
0.4684	-0.2946	0.9281	0.2465	0.1711	-0.07152	0.2705
0.2197	0.6154	0.664	-0.2237	0.1142	0.4312	0.1739
-0.3738	0.06452	-0.6483	0.02645	-0.5707	0.05456	-0.08758
0.6337	-0.08475	0.5282	-0.09988	0.0341	0.1518	0.1372
0.3409	-0.4098	0.3699	-0.3363	0.4911	-0.5861	-0.2674
0.3255	0.2327	0.1438	-0.2828	0.3803	0.02869	-0.4312
-0.6787	0.004656	-0.6727	0.1896	-0.4085	0.1274	-0.2739
-0.2165	0.3182	0.4933	-0.1734	0.02717	-0.5231	-0.1307
0.4477	-0.295	-0.5926	1.182	0.4392	-0.4422	-0.531
0.5695	-0.4013	0.4324	-0.155	0.4581	0.3847	0.7249
0.9326	-0.1025	-0.2503	-0.2865	0.4748	-0.08516	-0.5681
1.017	-1.004	0.4319	-0.4762	-0.5125	-0.7835	0.2143
0.8617	-0.4408	0.01345	0.007577	0.327	0.00624	-0.01169
0.05145	-0.7453	-0.2202	0.05212	0.3713	0.1716	-0.1218
-0.1097	-0.754	-0.2714	0.8172	-0.1574	-0.003711	0.09778
0.6882	-0.4449	-0.1205	-0.3691	0.0535	-0.4438	-0.1269
0.3854	-1.138	0.1975	-0.0509	0.1944	0.05809	-0.09903
-1.206	-0.1164	0.7606	-0.4549	-0.1955	0.3034	0.08448
0.4311	0.8988	0.4575	0.1391	-0.423	0.4918	0.05052
-1.217	0.7163	0.7552	-0.05105	-0.3965	0.6244	0.1927
0.3722	1.962	-0.905	0.3445	-0.2478	-0.53	-0.2329

-0.3337	1.305	0.5085	-0.4862	-0.1186	0.04461	0.1125
-0.6485	0.8228	-0.2835	-0.2462	-0.008126	-0.01625	-0.04163
-0.9812	0.08467	-0.02406	-0.1498	-0.3934	0.1116	-0.1707
-1.217	0.03783	0.424	-0.3104	-0.7016	0.4604	0.2473
-0.576	1.264	-0.4327	0.3649	0.1878	0.1357	0.04321
0.7415	0.6805	-0.7653	-0.3167	-0.2912	-0.372	0.5157
-0.1865	-0.5104	-0.7354	-0.5572	-0.4669	-0.3996	-0.2302
-0.6279	-0.5635	0.02822	0.37	-0.08094	0.7174	-0.784
-0.1777	-0.9915	0.2974	0.2148	0.09479	-0.359	0.1238
0.2185	-0.7286	0.6247	0.5719	-0.5029	0.4269	0.01415
0.6638	1.463	-0.2088	0.1851	0.6321	0.611	0.2399
-0.1193	0.1127	-1.58	-0.4883	0.3723	0.1726	0.5328
-0.5745	-0.8697	-0.4771	-0.2462	-0.3049	-0.569	0.5185
0.451	0.1431	0.01044	-0.1372	-0.8924	0.08573	-0.3046
-0.312	-0.6609	-0.8451	0.06329	0.02078	0.5737	0.3888
0.272	-0.595	-0.02699	0.6693	0.4297	0.43	0.09076
0.9172	0.8938	0.2663	-0.1265	0.1613	-0.4794	-0.1151
-0.7268	0.4436	0.6528	-0.5361	0.2123	-0.4173	-0.03364
-1.051	0.2094	0.02632	0.6906	0.5858	-0.2788	0.1446
-0.2486	0.4419	-0.2188	0.7842	-0.3914	-0.2832	-0.1223
0.153	0.01983	-0.4679	0.4359	-0.2296	0.1131	-0.04621
0.04484	-0.5021	0.5869	0.01422	0.9529	0.3237	0.0602
0.7574	0.3232	0.3595	-0.38	0.5556	0.3779	-0.09137
0.1914	0.01145	0.5982	0.639	-0.6525	0.3096	-0.07231
0.949	0.8873	-0.3265	0.01931	0.01972	0.4092	0.399
-0.869	0.6697	-0.6688	-0.7709	0.4788	-0.4068	-0.2816
-0.1376	0.6644	0.1587	-0.02474	0.2314	0.02138	0.03686
-0.7374	0.4914	0.4168	-0.2779	-0.2863	0.2054	-0.412
-0.9696	-0.1981	-0.4245	-0.4469	0.4405	-0.2	0.07189
-0.3242	0.2615	0.9797	0.1689	0.2173	-0.09438	0.02954
0.1751	0.8985	-0.0304	0.3084	-0.3171	-0.2725	0.05203
0.3345	0.2004	-0.4945	0.0444	-0.1734	0.1309	0.4273
-0.5238	-0.5505	-0.1726	0.8941	0.6578	0.3654	0.2188
-0.7738	-0.2249	0.4789	-0.1428	0.2417	-0.3157	-0.2807
-0.3479	0.2606	0.263	0.5051	0.3396	-0.5073	0.2677
0.8257	-0.1162	0.4079	-0.5346	0.05974	-0.1959	-0.1726

0.05583	-0.3497	0.01016	-0.2151	0.3916	-0.08124	0.1568
-0.07345	-0.9207	-0.5641	-0.7399	0.4073	-0.1322	0.06632
-0.6835	-0.02542	0.3653	0.4738	0.07724	-0.7578	0.2425
-0.4118	0.105	0.6054	0.829	0.1736	-0.1665	-0.2277
-0.2449	-0.01396	0.5207	-0.03187	0.2499	-0.2928	-0.2735
-0.4454	-0.2941	-0.1618	0.5006	0.005884	-0.4344	0.01727
-0.7852	-0.09914	-0.18	-0.1639	0.6204	0.1921	0.03551
-1.272	-0.02707	-0.43	-0.2969	0.1844	-0.2031	0.2089
0.8741	0.02499	-0.5421	0.1964	-0.2229	0.09388	-0.1773
0.4707	0.05451	-0.3569	-0.5132	0.3398	0.7907	-0.5985
0.6044	0.3139	0.3974	0.4572	-0.5774	-0.8192	0.2275
0.6254	0.4405	-0.03393	0.1131	-0.1112	-0.03053	0.1451
1.087	0.5538	0.5602	0.1215	0.05588	-0.09196	0.1202
-0.4028	-0.002958	-0.06084	-0.5936	-0.09436	0.09563	-0.1862
0.6074	-0.4913	-0.7547	0.2418	-0.1097	0.1083	0.2458
-0.3399	-0.2302	-0.9177	0.1368	-0.2545	0.1173	-0.2704
0.5124	-0.1298	0.1778	-0.208	-0.1816	0.2586	-0.1232
-0.4814	-0.4445	0.1823	-0.3832	-0.5009	0.105	0.1172
-0.000576	-0.9752	-0.3093	0.08595	-0.5074	0.1904	0.04467
0.2858	-0.6398	0.3307	-0.4579	-0.6306	-0.205	0.008531
0.6201	-0.07855	-0.05079	-0.3739	-0.2702	0.4525	0.2223
1.18	-0.1194	-0.1972	-0.2567	-0.2292	0.2107	-0.3479
0.118	-0.8736	0.2741	-0.2418	-0.2659	0.1197	0.0262
PC15	PC16	PC17	PC18	PC19	PC20	PC21
-0.08901	-0.3909	0.1151	-0.07955	-0.03116	-0.1228	-0.06373
-0.01418	0.4132	0.05759	0.1588	-0.08937	-0.1944	0.04602
0.3533	0.2374	-0.4119	0.05118	0.1848	0.07995	-0.0261
-0.06858	-0.3801	-0.111	0.0477	0.07232	0.115	0.006195
-0.3442	-0.07544	-0.0949	-0.2023	0.09652	0.1655	0.05539
-0.4015	-0.104	0.2412	-0.1882	0.00832	0.06566	0.1479
-0.1837	-0.3173	0.04666	-0.0899	-0.2093	0.06785	0.03186
0.6475	0.1455	-0.1826	0.1946	-0.1781	0.325	-0.0108
0.3938	0.02108	0.0379	-0.1264	0.1902	-0.09867	-0.01547
-0.1452	0.02574	-0.567	-0.4155	-0.04721	-0.01461	-0.3427
0.0135	-0.04435	0.09204	-0.04228	0.004947	0.1574	-0.03373
0.07155	-0.0608	-0.0329	-0.1196	0.35	0.02678	0.1792

-0.3441	-0.2029	-0.1642	0.2049	0.3234	0.2744	-0.1748
0.2103	0.05286	-0.4526	0.5472	-0.3521	-0.17	0.2886
0.5906	0.2	0.0503	0.04168	-0.4123	0.01973	0.06937
-0.2239	-0.08943	0.3134	0.008389	0.1526	0.1383	-0.03623
-0.03003	-0.1148	0.04532	0.2396	-0.2667	0.09097	-0.05734
0.4644	-0.1038	-0.1635	-0.2367	0.2183	-0.2191	0.1155
-0.07664	-0.008528	-0.0651	-0.1874	0.03351	-0.2053	-0.05467
0.07615	0.0412	0.5191	0.09946	0.01219	-0.04048	0.008012
0.007557	0.1866	0.162	-0.5256	-0.1138	0.1446	0.0604
0.04399	0.09344	0.02454	0.3434	0.1578	-0.1734	0.02168
-0.02732	0.1423	0.4505	0.3079	0.1147	0.2471	-0.09547
-0.3926	0.3125	0.151	-0.5727	-0.1961	-0.1443	0.01272
-0.3204	0.1899	-0.3491	-0.0155	0.1787	-0.2871	-0.1029
0.1438	-0.1575	-0.2091	0.1616	-0.2661	-0.09873	-0.1029
-0.002867	-0.07565	0.5261	0.1878	0.1921	0.1401	0.1556
-0.2647	0.6035	-0.2615	-0.06022	-0.05687	-0.04925	-0.001423
-0.03896	0.8098	0.03998	0.05308	0.4288	-0.07203	0.07307
-0.3019	-0.5598	0.08222	0.2979	-0.09938	0.1297	0.01774
0.434	0.3333	0.1819	-0.1538	0.08743	0.03939	0.07029
-0.07615	-0.2611	0.1077	-0.01593	0.09034	-0.09383	-0.0568
0.01399	0.1169	-0.5519	0.1389	0.02771	0.1222	-0.0244
-0.1078	-0.04447	0.03606	0.03389	-0.2052	-0.1471	-0.1868
-0.08007	-0.357	0.1179	-0.2181	-0.2362	-0.04571	0.1358
0.09816	-0.248	-0.2043	-0.1087	0.162	0.09663	0.003184
-0.07535	0.02807	0.1287	0.4048	0.04093	-0.1757	-0.08393
0.154	0.3032	0.1717	-0.04425	0.2004	-0.02205	0.01307
0.009679	-0.6339	0.2305	-0.1479	-0.1846	-0.215	-0.03705
0.3713	-0.0836	-0.2335	-0.08821	0.01534	0.1064	-0.01757
-0.3386	-0.177	-0.2145	-0.1483	-0.04556	0.1292	0.1404
0.2441	-0.0344	-0.03577	-0.114	-0.08085	0.0572	0.1101
0.02065	-0.09751	0.06329	-0.1093	0.1907	-0.1235	0.05755
-0.04963	0.01045	0.3624	0.1556	-0.1186	-0.147	-0.1621
-0.1163	0.08865	-0.1527	0.005171	-0.0664	0.08113	-0.01296
-0.2937	0.2965	0.01774	0.1218	-0.041	-0.08786	0.06582
-0.2289	-0.3647	-0.1277	0.01693	0.1172	-0.04502	0.05549
0.09115	0.0146	0.1377	0.1033	0.0005425	0.07176	-0.03084

0.5071	-0.1904	-0.1299	-0.07394	0.2029	0.04561	-0.07713
0.2636	0.2288	0.02889	0.04249	-0.1283	-0.135	-0.02432
-0.1747	0.1081	0.2449	-0.005784	0.004333	-0.005285	-0.06107
-0.5684	0.1156	-0.1649	0.02201	0.104	0.02299	0.08866
-0.3668	-0.005542	0.03421	0.05683	-0.148	0.1033	0.02271
0.4092	-0.4037	0.1429	-0.2511	0.08813	-0.1012	0.02494
-0.09018	0.1345	-0.06561	0.1363	0.127	0.1069	0.0801
-0.2033	0.0789	-0.03994	0.3417	6.91e-05	-0.01034	-0.1336
0.35	-0.01214	-0.04844	-0.07398	-0.0229	-0.1204	-0.00462
-0.07539	-0.1383	0.1433	0.1338	-0.05425	-0.1598	-0.0294
-0.0003466	0.003575	0.1137	-0.1749	0.1129	0.06731	-0.126
-0.1358	0.004602	0.1804	0.1246	-0.01304	0.01845	0.0444
0.4242	-0.1128	-0.06503	0.06254	-0.05104	-0.05522	0.0639
-0.1066	0.1128	0.0347	0.209	0.06262	-0.2071	-0.07565
0.3839	0.06923	0.01485	0.03149	-0.1411	0.1646	-0.1348
-0.328	0.2749	-0.01769	0.06908	-0.1096	0.1421	-0.007173
-0.1057	0.02894	-0.04196	-0.1916	0.05759	0.1278	0.02242
-0.1879	-0.4341	-0.3431	0.1411	0.1636	-0.1206	0.1101
0.08871	0.3088	0.3164	-0.2612	-0.1706	0.0417	-0.04964
0.1883	-0.005725	0.09259	-0.06379	0.1351	-0.08599	-0.03079
0.1506	-0.1479	0.2034	0.1719	-0.05275	-0.04138	-0.03354
0.2248	-0.0976	0.03585	-0.009834	-0.1447	0.1421	-0.03062
-0.2877	0.06507	-0.01801	-0.04435	-0.05199	-0.1071	-0.04396
0.004411	-0.3413	-0.0314	0.03393	0.2152	-0.1279	0.07976
0.325	-0.08489	0.09651	-0.0516	0.1441	0.07363	-0.051
-0.3302	0.1569	-0.05986	-0.06465	-0.2624	0.04916	0.05851
-0.3529	0.1854	-0.1964	-0.06276	-0.1587	0.03637	0.1139
0.1345	-0.06446	-0.2466	0.000851	-0.02571	0.04672	-0.03479
0.06192	0.1496	0.08871	0.0329	0.1088	0.03769	-0.03454
-0.04095	0.119	-0.04703	-0.04257	-0.2533	0.06859	0.04304
0.02167	-0.1902	-0.3168	-0.1268	-0.05514	0.0517	0.01131
0.09085	0.2777	0.1335	-0.1795	-0.1482	-0.02884	0.003416
-0.09118	0.1269	0.003111	0.1528	0.1105	0.06066	0.005165

PCA loadings

Table continues below

	PC1	PC2	PC3	PC4	PC5	PC6
C	-0.1225	0.1802	-0.02789	0.572	-0.06354	0.153
EC	-0.1722	-0.2174	0.2006	0.3945	-0.0381	0.2851
EGC	-0.0992	-0.3411	0.1276	0.08966	-0.3458	-0.1236
ECG	-0.06523	0.3303	-0.1095	0.1039	0.3518	0.3855
EGCG	-0.0861	0.01024	0.03225	-0.2691	-0.6305	0.4338
GA	0.08276	0.3676	-0.04787	0.09691	-0.3891	-0.0497
K	-0.2948	-0.03944	-0.239	-0.1335	0.1446	0.07328
Ca	0.279	0.2148	0.1233	0.1046	-0.2552	-0.1036
Mg	0.02214	0.2608	0.367	0.07261	0.1823	0.1029
Na	-0.009291	-0.337	0.2523	0.3345	-0.02702	0.111
Fe	0.352	-0.06376	-0.002897	0.08125	0.0157	-0.0009811
Mn	0.3647	-0.04493	-0.001845	-0.01035	-0.05789	0.07126
Cu	0.2459	0.2577	-0.1899	0.2374	-0.06207	0.1352
Zn	-0.1477	-0.0941	-0.4649	0.02793	-0.03017	0.3501
Pb	0.3356	-0.05005	-0.2194	0.06675	-0.01294	-0.07085
Cd	0.3145	-0.01163	-0.2916	0.08309	0.0297	-0.07283
Ni	-0.07371	-0.1924	-0.2333	0.4279	-0.01676	-0.314
Cr	0.2335	-0.04888	0.4393	-0.05398	0.2147	0.1375
TPC	-0.2028	0.3063	0.09774	0.0601	-0.1431	-0.3316
DPPH	-0.2001	0.3104	0.1196	0.076	-0.06573	0.01159
ABTS	-0.2643	0.1293	-0.006854	0.002457	0.03929	-0.3435

Table continues below

	PC7	PC8	PC9	PC10	PC11	PC12
C	-0.2614	0.01861	-0.2109	0.1018	-0.04301	0.1451
EC	-0.07752	-0.01537	-0.1606	0.2669	0.4172	-0.07096
EGC	-0.09184	0.06957	-0.1666	-0.479	-0.4096	0.08276
ECG	0.0189	0.01561	0.03028	-0.07068	-0.5795	0.2102
EGCG	0.2534	0.1778	0.1008	0.362	-0.1373	0.2286
GA	-0.01315	-0.03515	-0.1355	-0.08567	0.07963	-0.1916
K	0.2448	0.09521	-0.4467	0.03868	-0.07302	-0.4699
Ca	0.09222	0.07795	0.1738	-0.2315	-0.000938	-0.3244
Mg	0.5272	0.3362	-0.01864	-0.2003	0.1717	-0.02493
Na	0.07407	0.09227	0.1611	-0.06976	-0.2531	-0.2763
Fe	-0.2114	0.1505	-0.1312	0.03705	0.0185	0.247

Mn	-0.1528	0.1108	-0.1115	-0.001983	-0.01682	-0.1454
Cu	-0.004337	0.1253	-0.08248	-0.003911	-0.04575	-0.1902
Zn	-0.08587	0.2028	0.3378	-0.5288	0.3854	0.09725
Pb	0.01122	-0.07694	0.1651	0.1799	-0.07244	-0.03633
Cd	0.2209	0.09434	-0.09755	0.1111	0.04522	0.1419
Ni	0.5152	-0.05419	0.2605	0.1302	-0.0648	0.169
Cr	-0.004708	0.07559	0.1432	-0.03426	0.08365	0.191
TPC	0.06599	-0.03327	-0.2615	-0.1759	0.1426	0.4177
DPPH	-0.1076	-0.4417	0.4438	0.04685	-0.02398	-0.1857
ABTS	-0.3079	0.7165	0.2746	0.2618	-0.07569	-0.0877

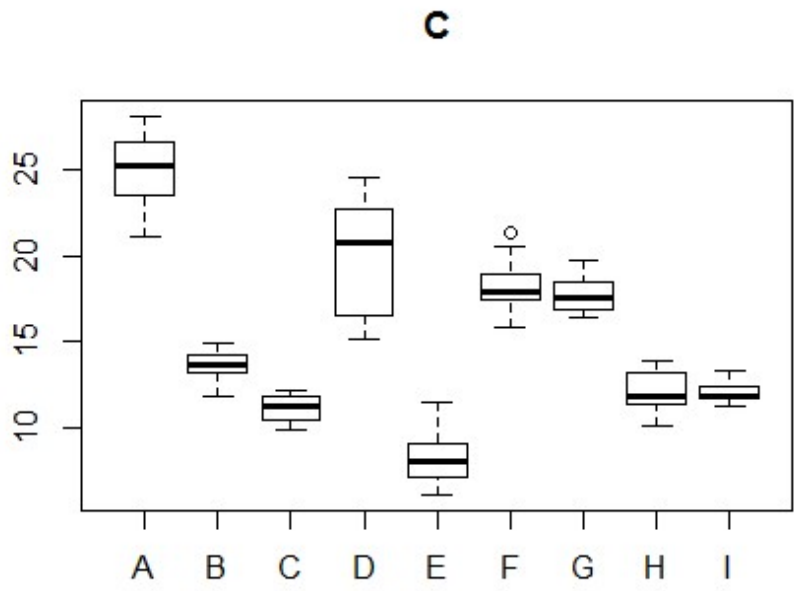
Table continues below

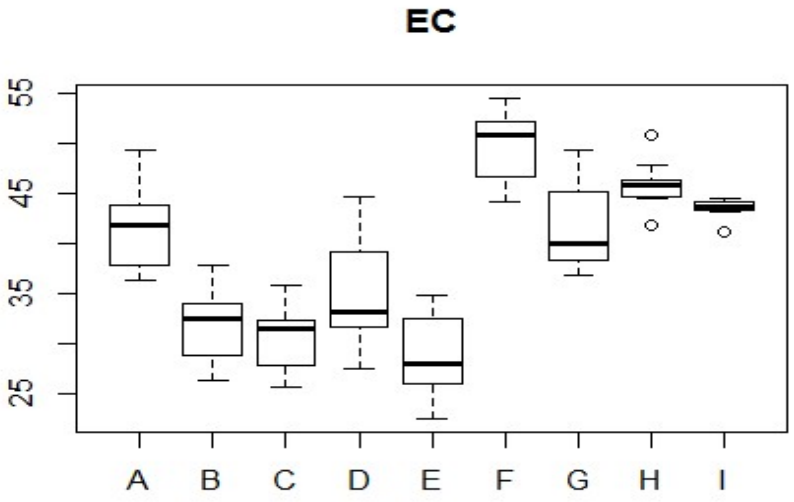
	PC13	PC14	PC15	PC16	PC17	PC18
C	-0.4978	0.2953	-0.01989	0.002446	0.1933	-0.259
EC	0.5425	0.012	0.1397	0.07777	-0.04616	0.1062
EGC	0.2018	0.1478	0.4153	-0.1319	-0.002578	-0.1124
ECG	0.3547	-0.03675	-0.09486	0.02369	0.01429	0.1416
EGCG	-0.1085	-0.04927	0.03444	0.07668	0.03549	-0.00485
GA	0.2276	-0.1173	-0.2795	-0.6241	0.1449	0.09083
K	-0.1688	-0.254	0.2392	-0.05486	0.3079	-0.007512
Ca	0.003448	0.1751	-0.08237	0.3261	0.003688	0.008235
Mg	-0.06997	0.2823	0.2295	-0.006642	0.04278	0.1697
Na	-0.1318	-0.4398	-0.3205	0.1845	0.02819	0.05555
Fe	-0.2533	-0.2115	0.272	-0.1428	-0.02364	0.6605
Mn	-0.03211	-0.1454	0.03667	0.1545	0.05949	0.02855
Cu	0.04323	-0.1873	0.1129	0.04606	-0.3506	-0.1655
Zn	-0.0409	-0.1051	0.0004101	0.005573	0.121	0.001402
Pb	0.2412	0.1578	0.1518	0.1812	0.714	0.01654
Cd	0.106	-0.1644	0.2684	0.04308	-0.2613	-0.4103
Ni	-0.05308	-0.0389	-0.04774	-0.2357	-0.01742	0.1184
Cr	-0.03	-0.3037	0.04804	-0.3564	0.2819	-0.4451
TPC	0.09758	-0.437	-0.06046	0.4141	0.1988	-0.001979
DPPH	-0.1065	-0.2336	0.5497	-0.01277	-0.03683	0.04157
ABTS	0.1193	-0.04281	0.0795	-0.04321	0.01657	-0.04151

	PC19	PC20	PC21
C	-0.04701	-0.08516	-0.03717
EC	0.1239	-0.1123	-0.02736
EGC	0.01303	0.06506	-0.00411

ECG	0.0739	-0.1814	-0.09797
EGCG	0.05058	0.00443	0.00146
GA	-0.2322	-0.07448	-0.01983
K	0.2067	-0.1509	0.02553
Ca	0.4325	-0.4821	0.08442
Mg	-0.295	0.169	-0.05111
Na	-0.3652	0.0007018	0.1666
Fe	0.08083	-0.1646	0.2104
Mn	-0.02782	0.1237	-0.848
Cu	0.2599	0.6007	0.2594
Zn	-0.01152	-0.02222	-0.02562
Pb	-0.1419	0.2097	0.2043
Cd	-0.3969	-0.4387	0.04771
Ni	0.3058	0.05551	-0.2492
Cr	0.3289	-0.04249	0.03531
TPC	0.02707	0.07662	-0.01014
DPPH	-0.1219	-0.04231	-0.1005
ABTS	-0.01532	-0.03106	-0.02899

Figure S2. Statistical significance of each parameter, separately.

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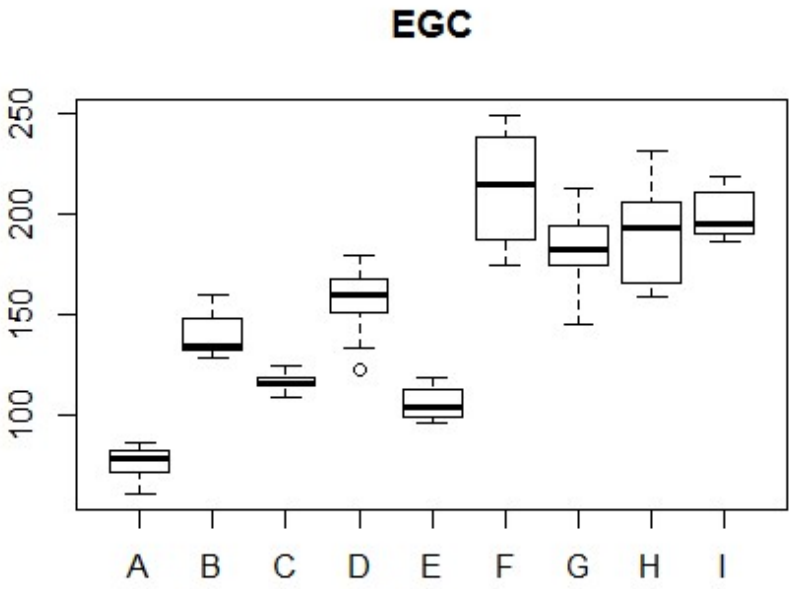
H
I


EGC
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100
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B
C
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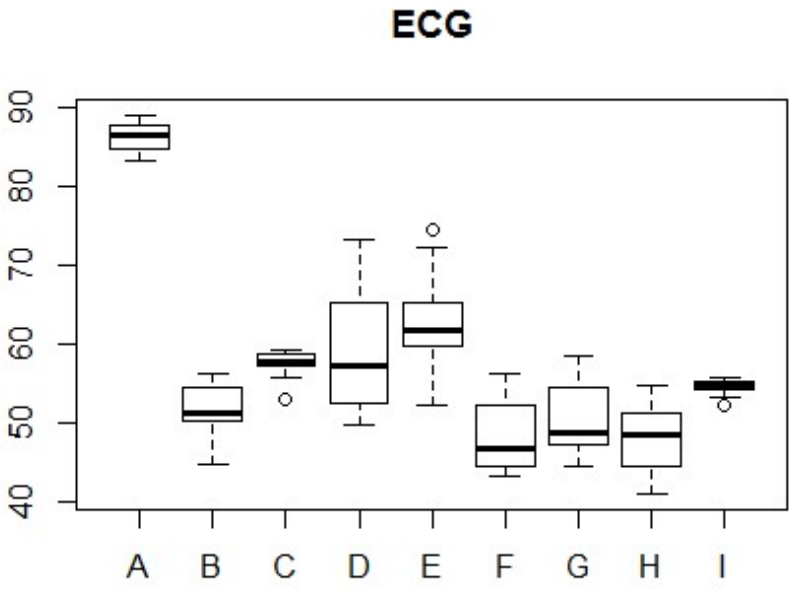
E
F
G
H
I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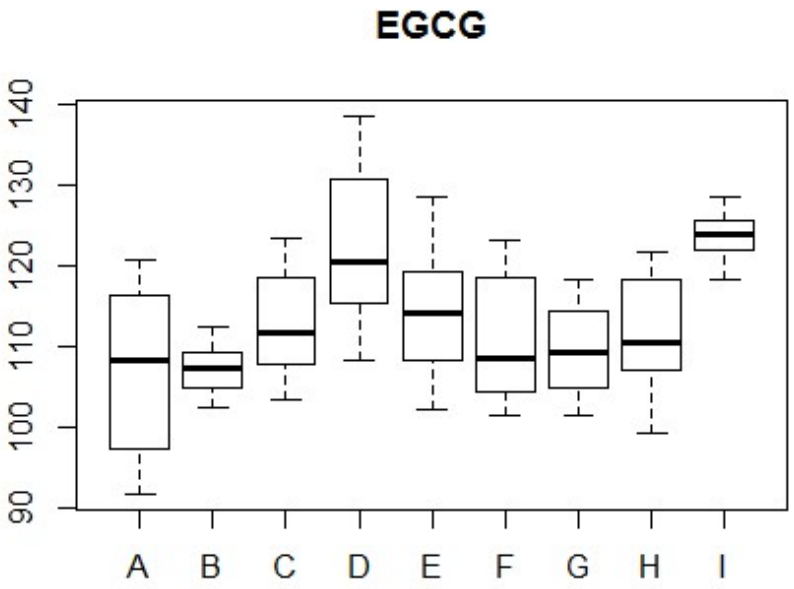
I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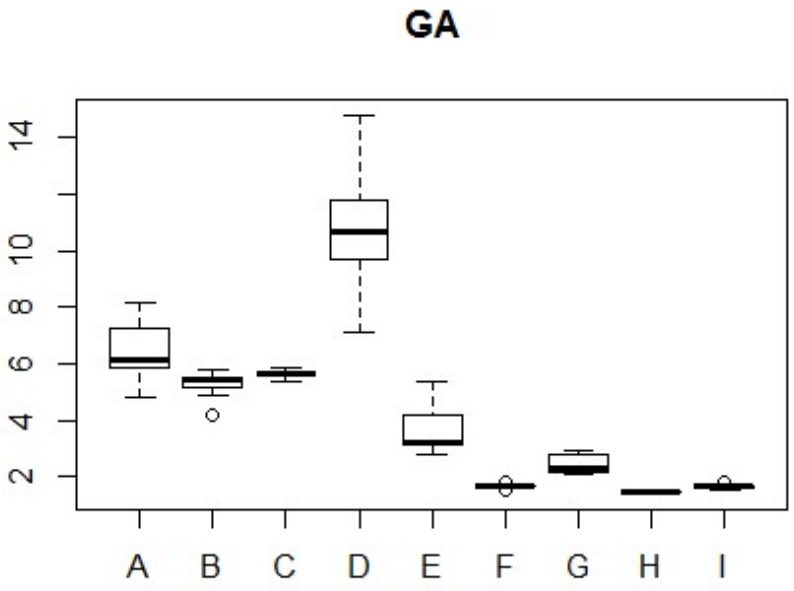
G
H
I


GA
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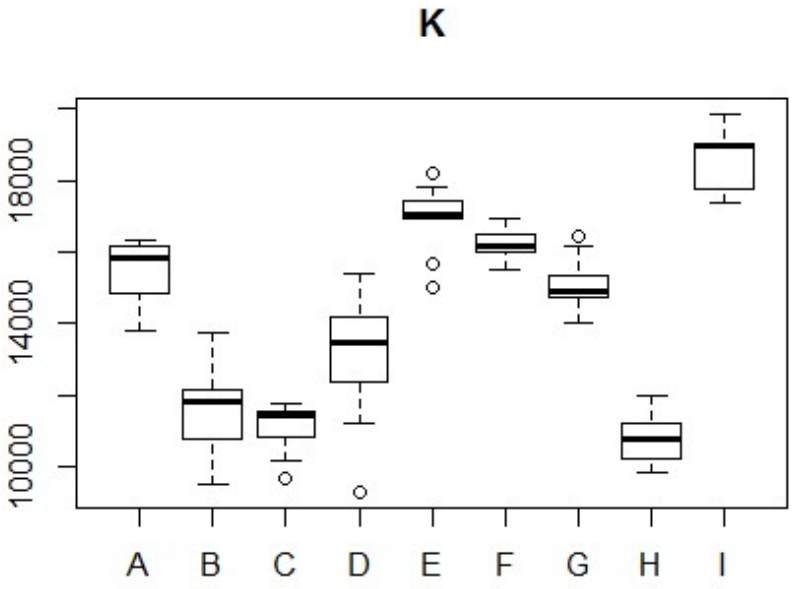
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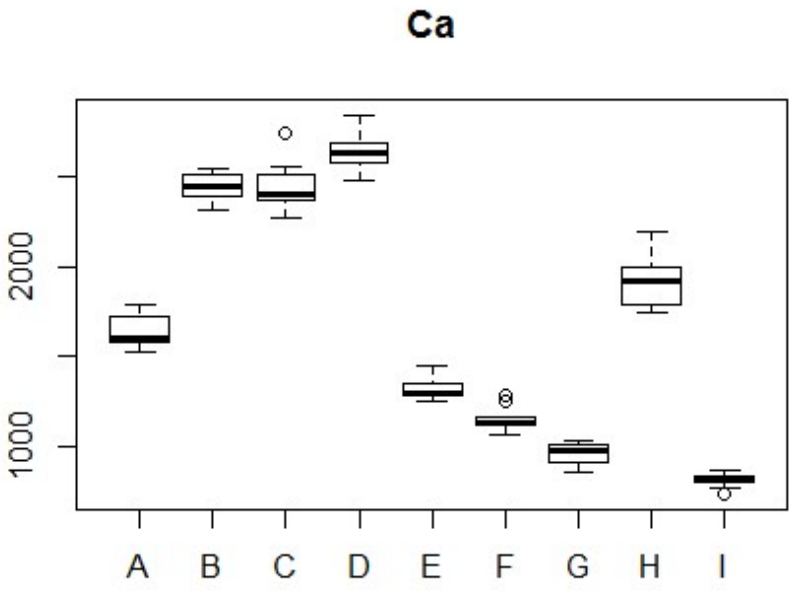
H
I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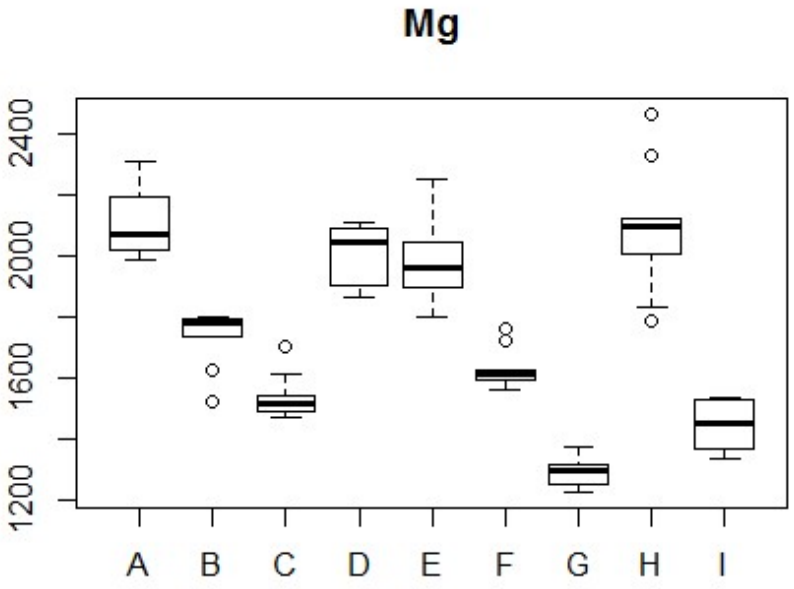
H
I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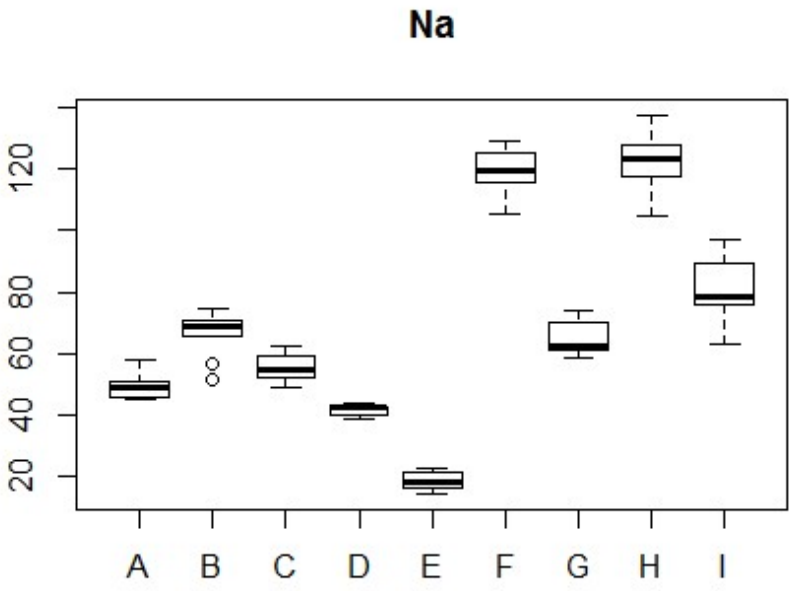
H
I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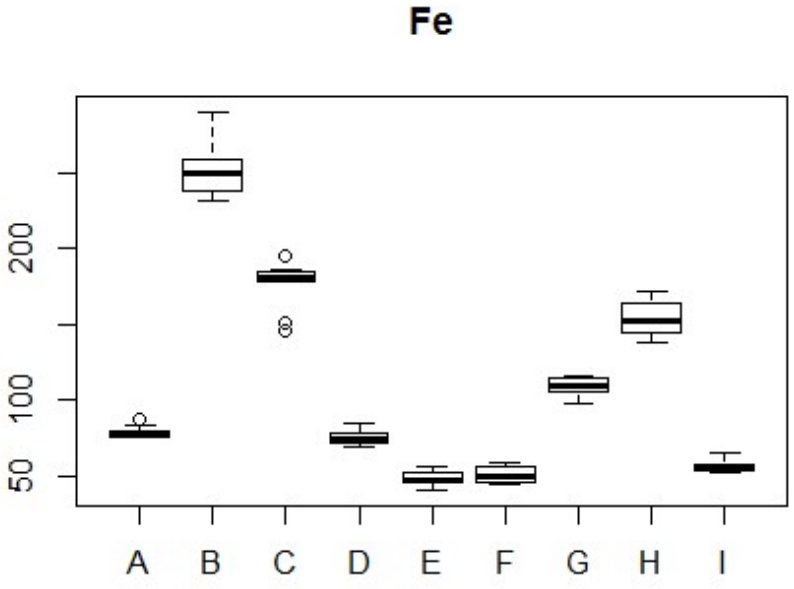
H
I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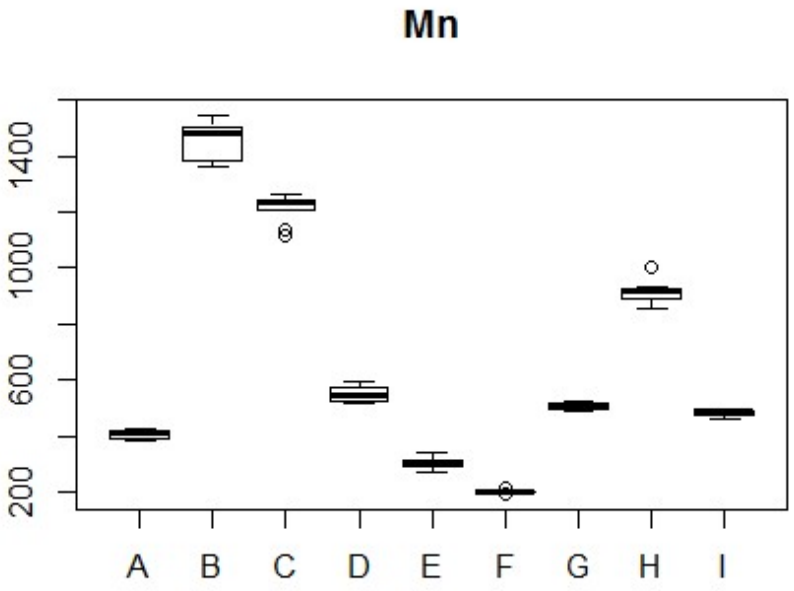
Mn
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600
1000
1400
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B
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D
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F
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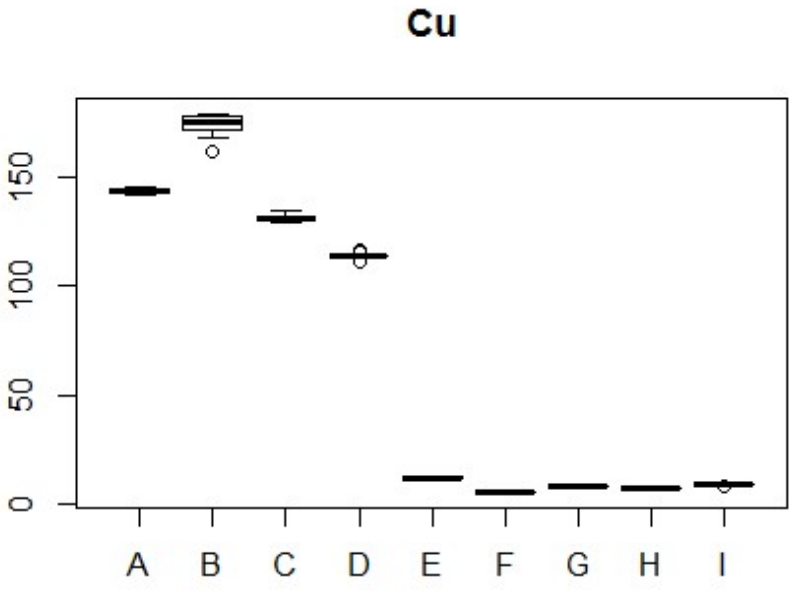
H
I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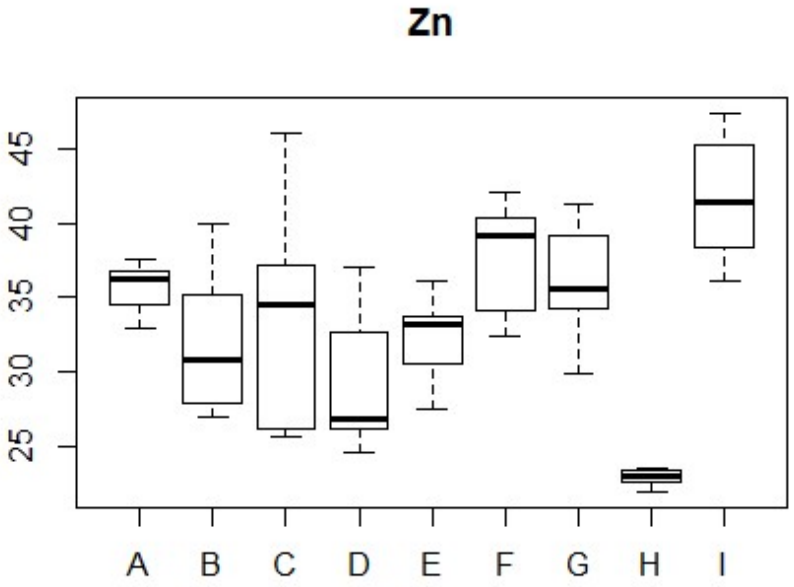
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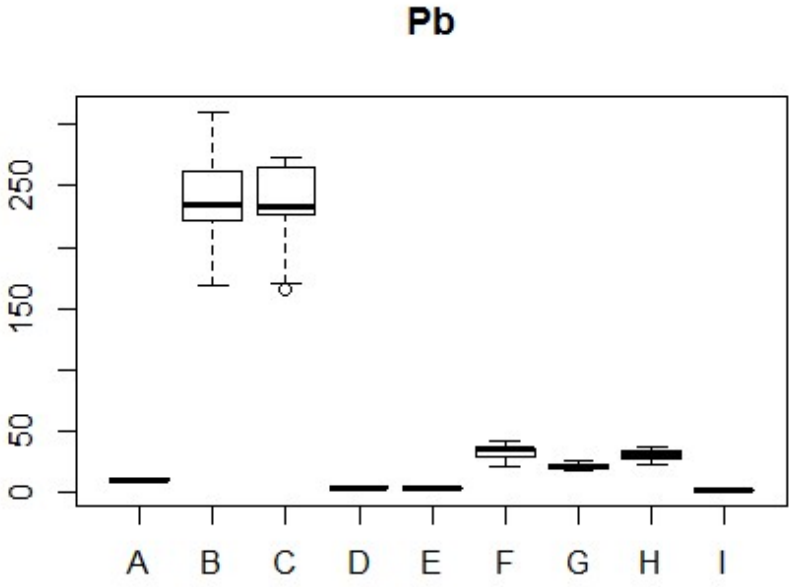
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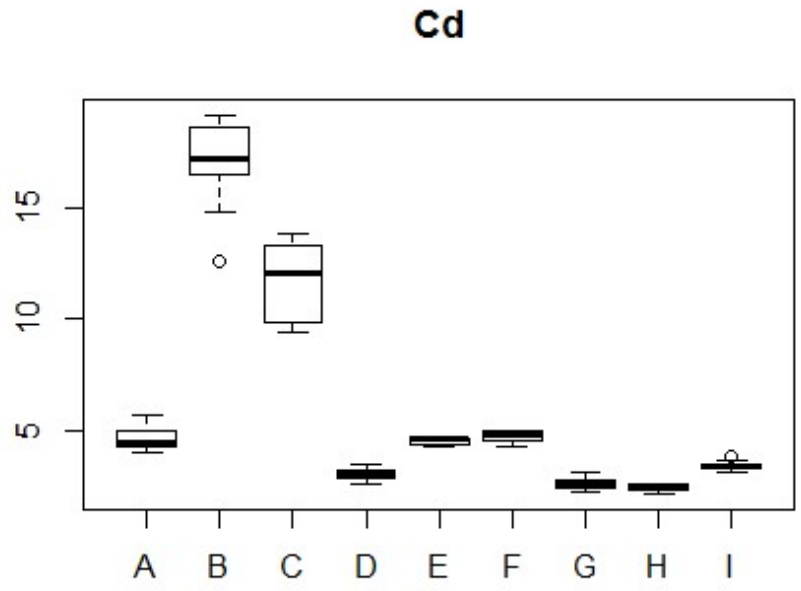
G
H
I


Cd
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15
A
B
C
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E
F
G
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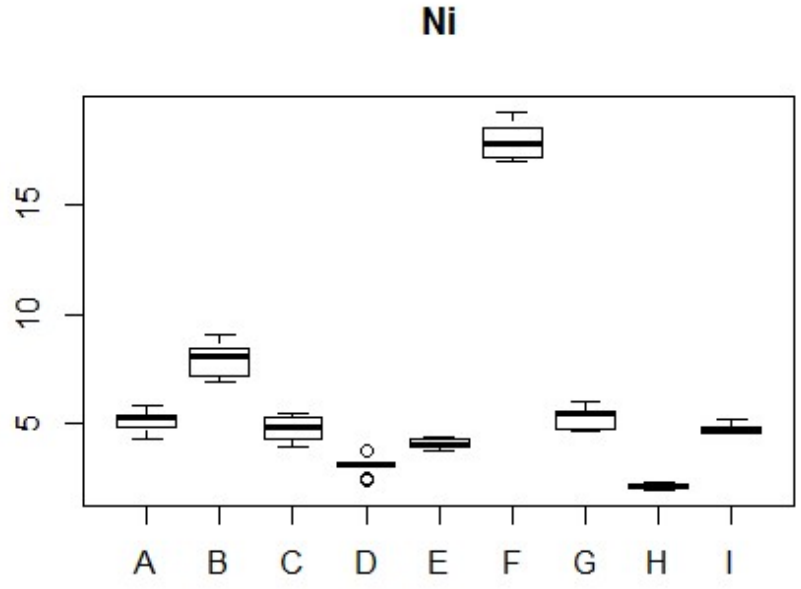
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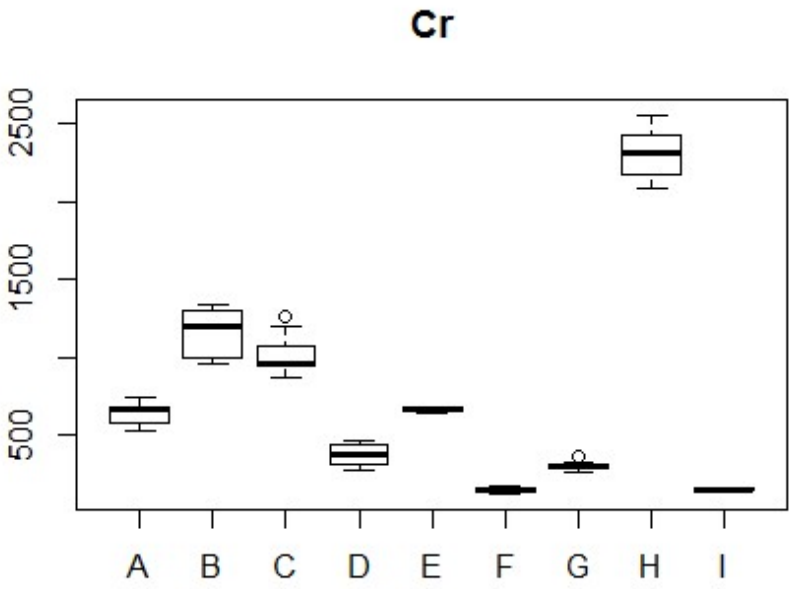
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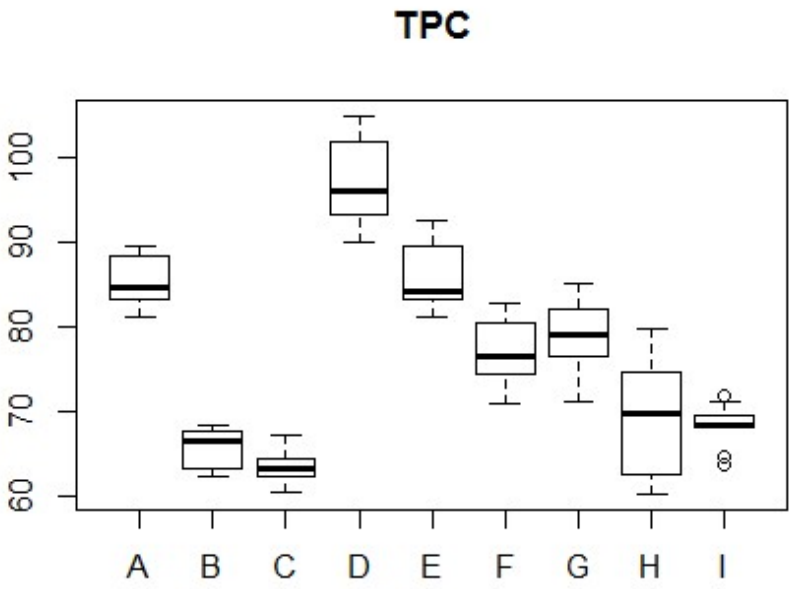
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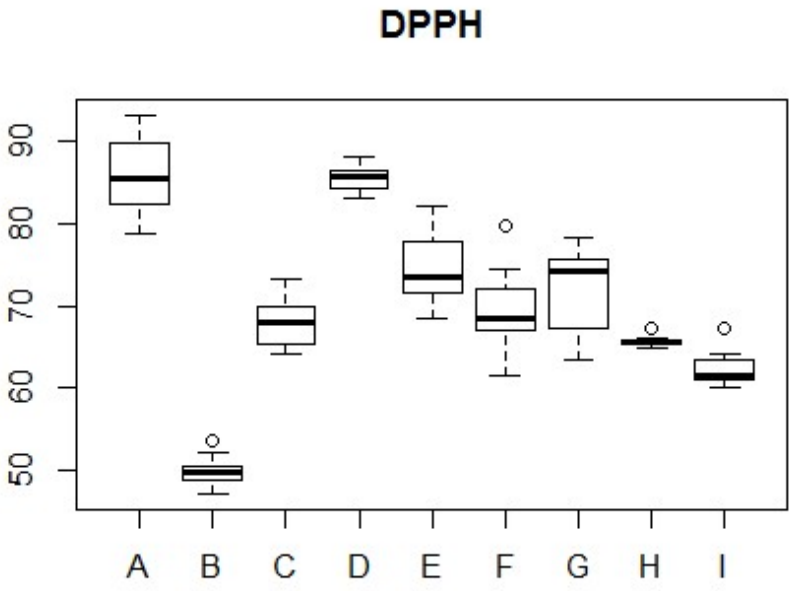
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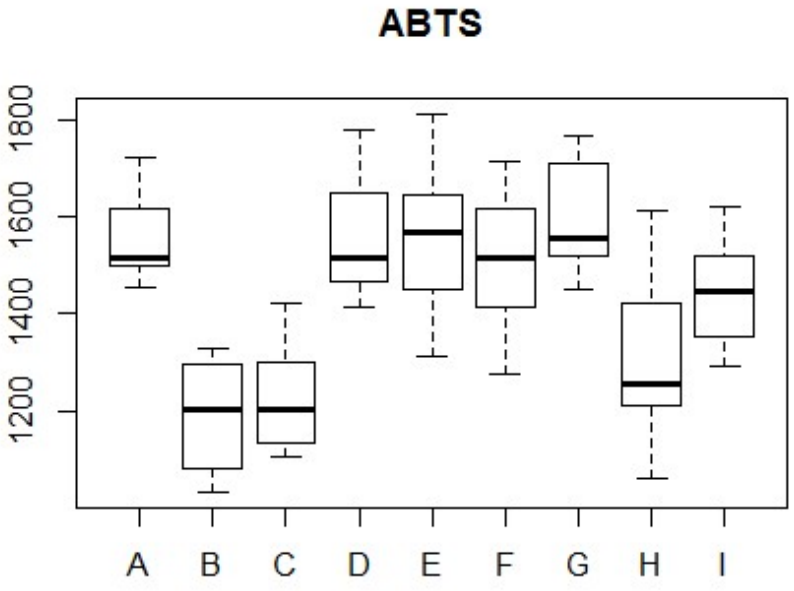
ABTS
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