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Anti-cancer Properties of Green Tea Probed Viaquantum Mechanics Calculations

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ABSTRACT

Tea, from the plant *camellia sinensis*, is consumed in different parts of the world as green, black or oolong tea. Among all of these, however, the most significant effects on human health have been observed with the consumption of green tea. Green tea contains polyphenols, which include flavanols, flavandiols, flavonoids, and phenolic acids. Most of the green tea polyphenols (GTPs) are flavonols, commonly known as catechins. There are four kinds of catechins mainly find in green tea: epicatechin, epigallocatechin, epicatechin-3-gallate, and EGCG. Green tea catechins have demonstrated significant antioxidant, anticarcinogenic, anti-inflammatory, thermogenic, probiotic, and antimicrobial properties in numerous human, animal, and *in vitro* studies. In the present study, four type catechins of green tea were studied. For each catechin ab initio method was employed for calculations and related parameters were computed.

Key words:DFT calculation, green tea,catechin, polyphenol, EGCG, antioxidant, anticarcinogenic.

INTRODUCTION

Tea is the most consumed drink in the world after water. Unlike black and oolong tea, green tea production does not involve oxidation of young tea leaves[1-3].

Green tea is produced from steaming fresh leaves at high temperatures, thereby inactivating the oxidizing enzymes and leaving the polyphenol content intact[4-8].

The polyphenols found in tea are more commonly known as flavanolsarcatechins, and comprise 30-40 percent of extractable solids of dried green tea leaves. The main catechins in green tea are epicatechin, epicatechin-3-gallate, epigallocatechin, and epigallocatechin-3-gallate (EGCG), with the latter being the highest in concentration[9-13].

Green tea polyphenols have demonstrated significant antioxidant,

Table 1: Results of optimize calculations for four catechins in green tea

Molecule	Energy (Kcal/mol)	Energy Gap (Kcal/mol)	Dipole moment	Quadrupole moment	Determinant of condensed to atoms	Determinant of Distance matrix
EC	-647167.1897	-126.9633	3.1259	-1508580	2.36359×10^{11}	1.55372×10^{11}
EGC	-694366.2589	-130.4898	4.0027	-1578059	1.1503×10^{12}	0
ECG	-1004872.918	-102.2144	3.6648	-5175210	1.51545×10^{18}	-3.98814×10^{15}
EGCG	-1052067.736	-106.9709	6.6295	-5568137	-	-

Table 2: Results of NMR calculations for(-)-epicatechin (EC)

Number of Atom	Atom	Isotropic	Anisotropy	Determinant of Magnetic Shielding Tensor	Determinant of Eigen value
1	C	40.7933	129.4848	-131534.6859	-132187.3863
2	C	101.1178	81.4917	749999.9317	749900.18
3	C	41.682	124.4068	-152111.1946	-152254.7644
4	C	98.2606	105.3572	618971.935	617123.4746
5	C	40.3898	119.5755	-120581.4747	-121553.1794
6	C	99.4788	96.0498	661610.9959	661291.5423
7	O	214.1367	53.5446	9450047.009	9443779.294
8	O	222.0782	73.8408	10461582.97	10407456.39
9	C	161.8983	16.4821	4221606.349	4220733.264
10	C	120.888	35.8661	1722200.697	1713626.209
11	C	109.2673	32.904	1268005.561	1267203.469
12	O	215.3092	78.6997	9240810.61	9165813.035
13	C	83.8394	109.1486	135341.9435	131769.2325
14	C	67.379	150.6034	-70446.14768	-72893.33234
15	C	75.7056	160.0222	-153597.7881	-153847.8002
16	C	78.9179	137.6591	49548.04689	47591.7128
17	C	51.6981	118.1888	-25234.30243	-28346.03287
18	C	55.7289	110.455	-14237.44592	-23269.86969
19	O	242.7435	37.6084	14057512.95	14048991.28
20	O	237.3366	93.0112	12686727.08	12634889.21
21	O	281.7297	78.6015	21839351.01	21763132.24
22	H	26.9099	4.8073	19130.43033	19130.05133
23	H	26.4725	6.6187	18050.67965	18048.18389
24	H	28.7916	12.6973	22036.45096	22029.18026
25	H	28.3778	11.2004	20559.56103	20549.31111
26	H	29.7656	7.1211	25573.39622	25558.2547
27	H	30.0048	6.6191	26405.99076	26383.14398
28	H	28.6196	2.3067	23414.05176	23383.86483
29	H	27.8962	5.8829	21344.96671	21343.94067
30	H	26.0539	8.5437	17044.42103	17039.40225
31	H	25.0369	9.2777	14899.52311	14898.21926
32	H	25.3491	5.0347	15942.47712	15938.84851
33	H	29.0284	13.5478	22369.32596	22348.95548
34	H	27.3461	12.1463	17802.84656	17801.49197
35	H	31.505	16.669	27807.03155	27649.59731

Table 3: NMR parameters for atoms of (-)-epicatechin (EC).

Number of Atom	Atom	ξ	Δσ	η	σ_{υ}^{iso}	σ_{σ}	Ω	S_{kew}	K	K
1	C	84.156	126.23	-0.18209	11.2354	42.078	161.819	118.572	0.922141	0.200732
2	C	53.2687	79.903	0.94402	8.93885	26.63435	106.8883	105.0464	0.041847	0.049599
3	C	80.6251	120.94	-0.5872	10.9972	40.31255	159.361	97.266	1.204514	0.12264
4	C	67.5861	101.38	-0.18875	10.0687	33.79305	123.3678	95.0006	0.976872	0.416034
5	C	78.0479	117.07	0.7984	10.82	39.02395	151.3926	148.2288	0.155895	0.159351
6	C	61.6544	92.482	-0.45074	9.61674	30.8272	118.563	78.5865	1.131609	0.240467
7	O	8.8715	13.307	1.82855	3.64791	4.43575	80.541	21.4183	-0.13689	-0.34075
8	O	47.5325	71.299	0.43347	8.44386	23.76625	98.9728	81.6006	0.408121	-0.01572
9	C	-1.8875	-2.8313	9.51862	1.68263	-0.94375	23.4801	-11.8145	1.027176	-0.19216
10	C	-8.0253	-12.038	-2.39641	3.46957	-4.01265	41.5035	-2.422	-0.98512	0.456677
11	C	-10.8911	-16.337	-0.52116	4.04186	-5.44555	35.0093	-13.4987	-0.70983	0.759458
12	O	27.5094	41.264	-2.61693	6.42371	13.7547	117.6908	5.2689	1.268148	-0.32521
13	C	-1.4625	-2.1937	-0.38359	1.48113	-0.73125	146.708	-1.9132	-0.02069	-0.02406
14	C	38.3435	57.515	2.94018	7.58388	19.17175	177.6133	113.8837	-0.62828	0.391714
15	C	29.6558	44.484	2.66408	6.66961	14.8279	196.6789	83.9864	-0.37637	0.254487
16	C	13.8435	20.765	1.98897	4.55689	6.92175	166.1593	34.5325	-0.12359	0.313907
17	C	27.3894	41.084	2.75265	6.40969	13.6947	137.3868	78.7808	-0.52411	0.441051
18	C	13.171	19.757	3.94475	4.44483	6.5855	133.6387	45.7347	-0.43534	0.30608
19	O	11.7717	17.658	1.29777	4.20209	5.88585	60.7981	25.2961	-0.08648	-0.52568
20	O	9.5707	14.356	2.27788	3.78894	4.78535	112.107	25.2565	-0.16364	0.318657
21	O	-21.752	-32.628	3.16183	5.71209	-10.876	91.3121	-67.016	0.772475	0.443199
22	H	-3.7979	-5.6969	-0.47718	2.38681	-1.89895	7.0941	-4.7907	-1.18624	-0.28947
23	H	-4.2122	-6.3184	0.53314	2.51362	-2.1061	8.7362	-7.4412	-0.33766	0.030494
24	H	-7.576	-11.364	1.22452	3.37105	-3.788	16.1426	-16.0026	0.158041	0.146278
25	H	-9.4737	-14.211	-0.15607	3.76969	-4.73685	17.036	-13.4712	-0.96433	-0.37017
26	H	-1.1455	-1.7183	2.33732	1.31082	-0.57275	10.2478	-3.057	0.224214	-0.22044
27	H	-1.4216	-2.1324	-0.56352	1.46027	-0.7108	9.1069	-1.7318	-0.36609	-0.0927
28	H	1.0056	1.5084	-0.43616	1.22817	0.5028	2.8266	1.2891	0.766398	0.264169
29	H	0.404	0.6061	-12.0666	0.77846	0.202	7.2332	-1.8314	1.094744	0.25329
30	H	-1.5179	-2.2768	5.17228	1.50892	-0.75895	9.8999	-6.2023	0.959585	0.452035
31	H	-2.4927	-3.7391	1.2588	1.93366	-1.24635	11.3719	-5.308	0.085078	0.263386
32	H	-1.9065	-2.8597	2.35337	1.69108	-0.95325	7.2825	-5.103	0.531493	-0.2346
33	H	1.4112	2.1169	0.12337	1.45492	0.7056	17.2437	2.2039	0.107622	0.142661
34	H	-2.0388	-3.0582	3.58245	1.74877	-1.0194	18.5115	-6.7101	0.426643	-0.3754
35	H	-9.5328	-14.299	1.12991	3.78143	-4.7664	21.6241	-19.6849	0.08589	0.083407

Table 4: Results of NMR calculations for (-)-epigallocatechin (EGC)

Number of Atom	Atom	Isotropic	Anisotropy	Determinant of Magnetic Shielding Tensor	Determinant of Eigen value
1	C	40.8019	129.4337	-131468.2548	-132109.6327
2	C	101.1489	81.4339	751314.675	751212.2715
3	C	41.7131	124.2695	-152261.0107	-152407.9893
4	C	98.2962	105.7753	617607.2076	615674.268
5	C	40.4762	119.3192	-120540.4738	-121470.4712
6	C	99.3432	96.1534	657786.1135	657460.7632
7	O	214.1095	53.6071	9447285.642	9440995.986
8	O	222.082	73.5106	10464384.51	10411199.43
9	C	161.9189	16.7679	4221685.215	4220717.894
10	C	121.4412	36.0943	1746115.875	1737920.775
11	C	109.415	32.5108	1274159.56	1273308.594
12	O	216.1166	80.7238	9325726.234	9246871.596
13	C	92.4905	96.9895	355343.3305	351557.0033
14	C	65.6881	155.1177	-80826.25932	-84441.42628
15	C	88.3958	130.7809	233168.3214	230188.5697
16	C	49.6752	118.0147	-27097.08213	-31945.97089
17	C	65.0882	97.6628	131362.7578	131304.7711
18	C	55.4935	108.5991	-1705.637668	-12467.12478
19	O	243.1531	36.5631	14126374.47	14117995.46
20	O	264.2844	85.8033	17851122.03	17824969.09
21	O	234.4268	97.6819	12142554.41	12089030.39
22	O	280.8084	78.6167	21625261.39	21543683.18
23	H	26.9056	4.7901	19115.63886	19115.18925
24	H	26.4412	6.7028	17974.30364	17971.87533
25	H	28.7934	12.7335	22032.02381	22024.99256
26	H	28.3798	11.1724	20558.6524	20548.90834
27	H	29.7438	7.1605	25504.48508	25490.06658
28	H	30.0328	6.5941	26474.82355	26451.09014
29	H	28.5931	2.2897	23351.60052	23320.64108
30	H	27.9385	5.6683	21457.45614	21456.58277
31	H	26.5138	7.8997	18034.92192	18029.56595
32	H	25.4382	9.8619	15572.96794	15568.46717
33	H	29.02	13.8912	22268.71786	22249.01053
34	H	27.8835	14.2057	18641.81058	18635.7062
35	H	27.2655	12.5265	17574.15693	17573.94869
36	H	31.3822	17.1506	27243.58921	27092.09421

Table 5: MR parameters for atoms of (-)-epigallocatechin (EGC)

Number of Atom	Atom	ξ	Δσ	η	σ_{υ}^{iso}	σ_{σ}	Ω	S_{kew}	K	K
1	C	78.1218	117.1828	-0.18838	10.8251	39.0609	161.7598	109.8245	0.860893	0.20064
2	C	50.4532	75.6798	1.064662	8.699414	25.2266	106.8064	102.5376	-0.04582	0.049778
3	C	73.5556	110.3334	-0.49137	10.50397	36.7778	159.2504	92.262	1.033261	0.121362
4	C	63.4072	95.11085	-0.15755	9.752477	31.7036	123.8494	90.116	0.888947	0.416257
5	C	73.4038	110.1057	0.921737	10.49313	36.7019	151.14	143.9352	0.057015	0.157848
6	C	55.9491	83.92365	-0.34519	9.160985	27.97455	118.6416	74.267	0.951552	0.24181
7	O	7.861	11.7915	2.967739	3.433875	3.9305	80.5013	23.4562	-0.28823	-0.33633
8	O	47.3016	70.95235	0.365588	8.423325	23.6508	98.6538	79.5988	0.456271	-0.01945
9	C	-3.8994	-5.84905	4.16877	2.418491	-1.9497	24.2159	-13.9769	0.76539	-0.23027
10	C	-8.6894	-13.0342	-2.76287	3.610277	-4.3447	41.2293	-1.0303	-1.18959	0.501808
11	C	-11.7969	-17.6954	-0.8198	4.206584	-5.89845	34.5894	-12.8598	-0.93098	0.759623
12	O	22.4023	33.60345	-3.3679	5.796848	11.20115	120.0135	-4.1209	1.223	-0.30951
13	C	14.9636	22.44535	-1.20394	4.737658	7.4818	134.1679	13.4377	0.368704	-0.10841
14	C	56.1754	84.26315	1.736677	9.179493	28.0877	181.4779	133.0424	-0.34205	0.418988
15	C	39.6574	59.4861	0.921286	7.712723	19.8287	157.1673	77.754	0.029792	0.32845
16	C	31.0505	46.5758	0.398151	6.824643	15.52525	136.8759	52.7572	0.204796	0.448808
17	C	31.8268	47.74025	1.41329	6.909428	15.9134	104.7299	70.2305	-0.18839	0.730084
18	C	27.9079	41.86185	1.277878	6.470073	13.95395	130.2724	59.6933	-0.08929	0.334526
19	O	14.2106	21.31585	1.457398	4.616915	7.1053	60.5023	31.6711	-0.16115	-0.5827
20	O	25.598	38.39695	0.491394	6.196531	12.799	95.8625	44.6863	0.203717	0.580269
21	O	33.7496	50.6244	1.940989	7.115083	16.8748	117.4906	83.3782	-0.40545	0.325609
22	O	-26.9131	-40.3697	2.543315	6.353712	-13.4566	91.6352	-74.5939	0.679904	0.431723
23	H	-3.5653	-5.34805	-0.4474	2.312564	-1.78265	7.128	-4.5505	-1.08598	-0.31191
24	H	-4.0246	-6.03685	0.575834	2.45701	-2.0123	8.8341	-7.1956	-0.28984	0.034978
25	H	-7.2942	-10.9412	1.300156	3.307764	-3.6471	16.181	-15.683	0.202979	0.147784
26	H	-9.036	-13.554	-0.15058	3.681576	-4.518	17.0343	-12.8737	-0.9155	-0.3765
27	H	0.046	0.06905	-87.5239	0.262679	0.023	10.3125	-1.944	0.59232	-0.22257
28	H	-2.5209	-3.78125	-0.72938	1.944569	-1.26045	9.141	-2.8619	-0.71536	-0.11447
29	H	0.7098	1.0648	-0.25951	1.031843	0.3549	2.7664	0.9727	0.484854	0.310801
30	H	0.1051	0.1577	-39.5243	0.397052	0.05255	7.1021	-1.9193	0.899565	0.192492
31	H	-1.5628	-2.34415	4.322818	1.531078	-0.7814	9.6201	-5.722	0.809711	0.284654
32	H	-3.8038	-5.70575	1.015747	2.388661	-1.9019	11.9462	-7.6376	0.007509	0.302079
33	H	-0.9209	-1.3814	-2.69606	1.175308	-0.46045	17.5854	-0.14	-0.29034	0.159712
34	H	-3.9819	-5.97285	1.326578	2.443941	-1.99095	20.2838	-8.614	0.096165	-0.1986
35	H	-6.1193	-9.17895	1.654748	3.029678	-3.05965	18.8294	-14.2419	0.319176	-0.33895
36	H	-9.6085	-14.4128	1.275652	3.796413	-4.80425	22.2449	-20.5413	0.178598	0.083952

Table 6: Results of NMR calculations for (-)-epicatechin-3-gallate(ECG)

Number of Atom	Atom	Isotropic	Anisotropy	Determinant of Magnetic Shielding Tensor	Determinant of Eigen value
1	C	40.4146	130.0009	-128615	-129298
2	C	100.8331	81.9869	741250.4	741138.7
3	C	41.7913	124.3387	-153638	-153693
4	C	99.2153	103.3459	650003.2	648009.2
5	C	40.915	119.5993	-126026	-127067
6	C	99.2005	96.3905	652721.2	652351.4
7	O	213.5399	53.3362	9356683	9350524
8	O	221.7059	73.539	10412724	10360978
9	C	161.8432	18.892	4216965	4215851
10	C	111.9613	50.4775	1313604	1307693
11	C	112.7245	38.8766	1381136	1378868
12	O	217.6278	74.2272	9588378	9507721
13	C	76.6871	131.5557	19844.72	16156.17
14	C	69.8138	147.6212	-58409.9	-59125.5
15	C	76.2222	161.6723	-148429	-149378
16	C	81.184	135.6802	84354.25	81708.69
17	C	50.9251	121.5665	-30327.8	-35385.4
18	C	55.4857	109.741	-26581.9	-34220.8
19	O	251.2283	40.5396	15622818	15483215
20	O	239.1597	93.2347	13003724	12931497
21	O	134.0707	145.1335	-390236	-520509
22	C	73.6342	135.9389	-30737.7	-30908.9
23	C	87.8734	125.3321	272625.8	271983.8
24	C	52.5862	115.2903	-7435.83	-11267.4
25	C	61.3147	103.8535	86001.26	85805.84
26	C	54.2027	111.3854	-21345.3	-28559.7
27	C	86.7742	116.5835	205590.6	204884
28	C	26.4825	77.4218	-280606	-283156
29	O	-95.4139	579.7699	21461495	21461917
30	O	242.1249	32.4512	13923375	13917987
31	O	257.1364	98.1199	16228249	16212366
32	O	236.9415	93.018	12635932	12574274
33	H	26.8644	4.9382	19019.39	19018.64
34	H	26.4448	6.8991	17956.37	17954.87
35	H	28.7275	12.7808	21858.77	21851.09
36	H	28.3537	10.9946	20603.79	20594.37
37	H	29.4838	5.8049	24661.02	24656.26
38	H	29.597	6.1079	25334.84	25314.18
39	H	27.8979	7.5734	21136.99	21132.83
40	H	27.4551	4.8791	20439.09	20427.47
41	H	25.3289	8.1221	15747.41	15729.67
42	H	25.2434	8.55	15354.62	15352.9
43	H	25.6134	4.1254	16523.21	16517.52
44	H	28.4687	13.8161	20973.78	20906.58
45	H	27.2212	11.594	17655.35	17645.91
46	H	25.9561	7.9531	16842.7	16840.41
47	H	26.398	7.1822	17910.92	17902.09
48	H	28.9066	13.5722	22041.84	22012.07
49	H	27.603	13.8326	18078.81	18073.67
50	H	27.4441	13.1068	17888.99	17888.06

Table 7: NMR parameters for atoms of (-)-epicatechin-3-gallate(ECG)

Number of Atom	Atom	ξ	Δσ	η	σ_{υ}^{iso}	σ_{σ}	Ω	S_{kew}	K	K
1	C	7.7267	11.59	9.05305	3.404416	3.86335	162.0315	46.5651	-0.57603	0.209274
2	C	22.278	33.41705	1.788953	5.780744	11.139	107.2141	53.3442	-0.2459	0.058811
3	C	-2.6713	-4.00695	1.370232	2.001737	-1.33565	159.4497	-5.8371	0.009304	0.119197
4	C	5.8784	8.81755	9.744165	2.969444	2.9392	121.788	37.4576	-0.63309	0.394288
5	C	29.5938	44.39065	1.741449	6.662635	14.7969	152.0694	70.1587	-0.21644	0.145913
6	C	2.9236	4.3854	0.24162	2.094135	1.4618	118.9195	4.7386	0.027967	0.242208
7	O	6.9321	10.3982	-4.5467	3.224616	3.46605	81.3503	-5.3609	0.708978	-0.37746
8	O	4.7054	7.0581	14.8775	2.656708	2.3527	98.3336	42.0604	-0.99609	-0.00859
9	C	-1.8499	-2.77485	11.26747	1.665788	-0.92495	24.0225	-13.1967	1.186001	0.145713
10	C	11.7206	17.5808	-0.75991	4.192958	5.8603	58.8536	13.1275	0.52572	0.430715
11	C	8.5376	12.80635	-2.58099	3.578603	4.2688	41.6497	1.7886	1.101076	0.733669
12	O	-13.7643	-20.6465	-0.06029	4.543836	-6.88215	114.3566	-20.2316	-0.19143	-0.40366
13	C	-73.8572	-110.786	-0.71229	10.52548	-36.9286	162.8586	-84.4818	-1.1648	0.231162
14	C	-23.642	-35.463	-3.85252	5.955082	-11.821	175.4798	10.0776	-0.98065	0.364974
15	C	-52.0949	-78.1423	-1.63112	8.839816	-26.0475	197.8733	-35.6558	-1.03906	0.268199
16	C	-69.9258	-104.889	-0.92698	10.24152	-34.9629	164.2612	-72.4789	-1.23047	0.30401
17	C	-26.3827	-39.5742	-3.63959	6.290791	-13.1914	140.9664	8.437	-1.30249	0.449518
18	C	-41.8018	-62.7028	-1.59108	7.918504	-20.9009	134.7094	-29.4477	-1.20606	0.258599
19	O	-6.8938	-10.3408	-6.3382	3.215696	-3.4469	69.9408	11.5064	-1.08495	-0.68149
20	O	-48.6136	-72.9203	-0.62643	8.539344	-24.3068	112.7584	-57.6938	-1.0518	0.307414
21	O	-29.9409	-44.9113	0.230868	6.701593	-14.9705	243.1042	-48.3675	-0.14209	-0.61199
22	C	17.1075	25.66125	-2.07715	5.065693	8.55375	167.4073	7.8938	0.471686	0.248097
23	C	27.0472	40.57075	0.895586	6.369521	13.5236	148.5328	52.6823	0.028519	0.375204
24	C	35.4432	53.1648	-0.54705	7.29142	17.7216	132.2442	43.4702	0.621945	0.487194
25	C	23.796	35.694	-0.58152	5.974446	11.898	111.3008	28.7751	0.50719	0.732353
26	C	29.1516	43.72735	0.841618	6.61267	14.5758	134.0537	55.9946	0.051662	0.323604
27	C	40.0594	60.08905	-0.54034	7.751716	20.0297	148.9894	49.2662	0.621235	0.129982
28	C	28.8574	43.28615	2.506529	6.579217	14.4287	137.6393	79.4521	-0.47379	-0.75001

29	O	117.1788	175.7682	3.147341	13.25776	58.5894	677.7678	360.169	-0.55688	0.421644
30	O	1.754	2.63095	-25.4857	1.622036	0.877	59.5717	-19.72	1.169745	-0.82104
31	O	31.2182	46.8273	-0.16102	6.843048	15.6091	108.3932	44.3139	0.501577	0.620887
32	O	19.7094	29.564	0.386202	5.437288	9.8547	111.6856	33.3699	0.162475	0.331421
33	H	-0.1476	-0.22135	18.0332	0.470532	-0.0738	7.2399	-1.5522	0.520905	-0.27166
34	H	-1.4491	-2.1736	3.908909	1.47433	-0.72455	9.0483	-5.0058	0.698816	0.049932
35	H	-3.8015	-5.70225	2.29612	2.387938	-1.90075	16.2467	-10.0666	0.454911	0.14667
36	H	-0.1741	-0.2612	49.3498	0.511028	-0.08705	16.6867	-4.5571	0.756674	-0.36446
37	H	-6.1554	-9.23305	-0.15919	3.038602	-3.0777	10.2434	-8.7431	-1.04485	-0.7332
38	H	3.9092	5.8639	-1.06984	2.421528	1.9546	8.8922	3.7728	1.364949	-0.25246
39	H	-3.9213	-5.8819	0.377885	2.425273	-1.96065	9.1175	-6.6228	-0.40133	0.322621
40	H	-0.3428	-0.5142	2.590432	0.717077	-0.1714	6.2578	-0.9582	0.130685	0.118748
41	H	-2.7662	-4.1493	0.152411	2.036983	-1.3831	8.4288	-4.3601	-0.41725	0.854428
42	H	1.8959	2.84385	-2.75811	1.686372	0.94795	10.8534	0.2293	0.984714	0.151059
43	H	0.7213	1.082	-4.31415	1.040168	0.36065	6.3933	-0.4739	0.899348	-0.41894
44	H	5.5854	8.3781	0.166219	2.894495	2.7927	17.6377	8.8423	0.396055	0.1333
45	H	5.6924	8.53865	-1.35048	2.922088	2.8462	17.9692	4.6949	1.116911	-0.41913
46	H	-4.1296	-6.19445	-1.0733	2.488855	-2.0648	10.045	-3.9783	-1.27855	0.166979
47	H	-2.2334	-3.3501	0.128235	1.830328	-1.1167	8.6481	-3.4933	-0.3377	0.321955
48	H	-6.0857	-9.1285	-0.69704	3.021349	-3.04285	17.3869	-7.0075	-0.89098	0.122385
49	H	-4.5332	-6.79985	0.994728	2.607643	-2.2666	19.984	-9.0545	-0.0018	-0.23128
50	H	-3.5282	-5.2924	-0.91457	2.3005	-1.7641	19.2772	-3.679	-0.52564	-0.28036

Table 8: Results of NMR calculations for(-)-epigallocatechin-3-gallate (EGCG)

Number of Atom	Atom	Isotropic	Anisotropy	Determinant of Magnetic Shielding Tensor	Determinant of Eigen value
1	C	40.4524	129.862	-128713	-129210
2	C	99.6995	97.8347	676158.5	676097.1
3	C	40.8537	125.5443	-150525	-150577
4	C	98.7956	103.4706	637057.1	635174.6
5	C	41.047	119.6756	-118159	-119400
6	C	100.695	80.7105	723196.7	722809.2
7	O	213.9399	53.9164	9400224	9396174
8	O	220.4964	75.2578	10202384	10154243
9	C	160.964	18.3701	4151548	4150085
10	C	113.5261	46.8777	1384243	1380054
11	C	108.7181	29.8684	1254469	1252936
12	O	208.8412	80.9209	8390864	8313384
13	C	84.4214	114.0603	180000.3	175519.3
14	C	59.3692	169.6506	-128925	-129874
15	C	91.1127	127.0327	294166.5	289658.6
16	C	46.6936	124.9664	-61746.4	-67766.5
17	C	67.5615	77.3282	182209.5	182107.1
18	C	46.7106	125.4811	-52114.6	-58828.3
19	O	232.0068	88.4187	11894662	11819705
20	O	293.5939	134.5975	23578633	23572063
21	O	146.9444	139.5594	368775	232676.1
22	C	72.5049	136.8501	-45651.7	-46046
23	C	87.5227	125.3313	270600.4	269816
24	C	52.3823	115.2445	-8546.29	-12662.3
25	C	61.6343	103.0269	89737.44	89581.53
26	C	54.2623	110.6945	-19111.6	-26408.3
27	C	86.6519	116.3523	202793.9	202173.4
28	C	29.034	73.9967	-308911	-311190
29	O	-113.032	608.4679	26112351	26162998
30	O	242.1023	34.3492	13928407	13925118
31	O	257.8886	96.3126	16400978	16385666
32	O	236.9009	92.7637	12632903	12572243
33	O	234.9932	86.0768	12395803	12319916
34	H	26.375	4.6461	17990.46	17990.01
35	H	27.0259	7.2398	19184.59	19182.48
36	H	28.8042	11.8772	22132.24	22128.13
37	H	28.3005	10.5617	20584.77	20573.15
38	H	29.5952	6.026	25423.05	25397.77
39	H	29.4205	6.287	24434.1	24432.15
40	H	27.6734	7.3151	20627.26	20607.36
41	H	27.7448	6.1196	21005.79	20999.58
42	H	25.8174	7.5733	16683.84	16677.62
43	H	26.0377	7.9109	17139.27	17134.88
44	H	27.475	12.1494	18314.9	18302.09
45	H	30.5854	18.0495	25722.42	25644.91
46	H	25.796	8.0162	16510.66	16504.99
47	H	26.2549	6.6232	17688.98	17686.58
48	H	28.9466	13.7936	22118.84	22094.03
49	H	27.6021	13.9758	18055.48	18050.28
50	H	27.4034	13.024	17806.56	17805.54
51	H	27.3753	12.8376	18048.34	18031.36

Table 9: NMR parameters for atoms of(-)-epigallocatechin-3-gallate (EGCG)

Number of Atom	Atom	ξ	Δσ	η	σ_{υ}^{iso}	σ_{σ}	Ω	S_{kew}	K	K
1	C	2.1076	3.16145	29.93049	1.778033	1.0538	161.8811	34.7022	-0.56499	0.208824
2	C	19.6453	29.468	2.505811	5.428439	9.82265	117.8673	54.0817	-0.37647	0.320165
3	C	-1.4016	-2.10235	-1.10295	1.449966	-0.7008	160.3287	-1.3294	-0.02758	0.132173
4	C	4.0243	6.03645	14.54621	2.456919	2.01215	122.161	35.3056	-0.66937	0.38801
5	C	28.4815	42.7223	2.266089	6.536226	14.24075	151.1318	74.9931	-0.3579	0.167451
6	C	-1.0614	-1.59215	8.173639	1.261784	-0.5307	108.4029	-5.9299	0.105357	-0.02183
7	O	13.3067	19.96005	-1.07807	4.467667	6.65335	82.223	12.7873	0.504461	-0.37707
8	O	2.9906	4.4859	23.78145	2.117994	1.4953	101.1382	40.0463	-1.01045	-0.02356
9	C	-2.8619	-4.2929	7.220029	2.071919	-1.43095	22.3546	-14.6244	1.194452	0.287028
10	C	11.2068	16.81015	-0.69214	4.100024	5.6034	54.1057	12.9318	0.525732	0.465633
11	C	8.4506	12.676	-2.09862	3.560323	4.2253	33.5169	3.8087	1.171889	0.564584
12	O	-15.7736	-23.6604	2.104992	4.864196	-7.8868	118.8752	-40.262	0.219934	-0.27711
13	C	-31.2013	-46.802	-0.77024	6.841195	-15.6007	146.6063	-34.7857	-0.56513	0.112014
14	C	3.0813	4.62205	20.43524	2.149872	1.54065	197.2363	36.1056	-0.45544	0.440555
15	C	-17.3201	-25.9802	-0.50765	5.097073	-8.66005	154.0645	-21.5839	-0.25424	0.298169
16	C	-28.2848	-42.4272	-1.17083	6.513617	-14.1424	148.3468	-25.8688	-0.62086	0.369573
17	C	2.6797	4.01965	15.0144	2.004882	1.33985	92.0648	24.1367	-0.61187	0.35973
18	C	-10.2306	-15.346	-0.69883	3.917384	-5.1153	147.2781	-11.7712	-0.17701	0.408004
19	O	-9.2584	-13.8876	-4.52504	3.726607	-4.6292	108.3139	7.0597	-0.7084	0.265276
20	O	-26.3268	-39.4902	-0.00725	6.284123	-13.1634	153.8865	-39.3948	-0.25848	0.498619
21	O	-21.8775	-32.8163	0.119095	5.728547	-10.9388	235.0348	-34.119	-0.12299	-0.62487
22	C	20.744	31.11605	-2.16804	5.578172	10.372	168.539	8.6291	0.584891	0.247915
23	C	27.1654	40.74805	0.968419	6.383424	13.5827	148.036	53.9018	0.008692	0.386511
24	C	37.4295	56.1442	-0.32061	7.492947	18.71475	132.3643	50.144	0.560156	0.482648
25	C	26.4265	39.6398	-0.56766	6.296011	13.21325	110.6064	32.1392	0.561827	0.725896
26	C	28.8434	43.26505	1.016243	6.577621	14.4217	133.2275	57.921	-0.00528	0.323474
27	C	41.8076	62.71145	-0.23453	7.919053	20.9038	148.9132	57.8089	0.519895	0.125374

28	C	27.0938	40.64065	1.719917	6.375006	13.5469	137.164	63.9402	-0.21331	-0.84209
29	O	162.9905	244.4857	2.257987	15.63604	81.49525	710.2157	428.5009	-0.43305	0.426947
30	O	3.8489	5.77335	-12.2465	2.40278	1.92445	59.9098	-17.7944	1.276529	-0.7066
31	O	31.7812	47.67175	-0.02395	6.904477	15.8906	106.646	47.2912	0.457713	0.61242
32	O	21.2588	31.88825	0.087357	5.646964	10.6294	111.3073	32.8168	0.261463	0.333609
33	O	4.1999	6.2998	3.659182	2.50995	2.09995	106.646	13.9839	-0.15709	0.228504
34	H	-0.085	-0.1275	27.89176	0.357071	-0.0425	7.084	-1.3129	0.484006	-0.37657
35	H	-1.2965	-1.94475	4.328346	1.394543	-0.64825	9.1239	-4.7506	0.709433	0.174005
36	H	1.0761	1.6142	0.496794	1.270492	0.53805	15.7111	1.8815	0.051709	0.023907
37	H	0.1371	0.20565	-61.5529	0.453486	0.06855	16.2117	-4.0138	0.793501	-0.39407
38	H	3.8433	5.765	-0.95428	2.401031	1.92165	8.3525	3.9312	1.348878	-0.11418
39	H	-6.3795	-9.5693	-0.21936	3.09342	-3.18975	10.732	-8.8696	-1.08726	-0.65672
40	H	-3.6605	-5.49075	0.285453	2.343235	-1.83025	9.2409	-6.0132	-0.42457	0.166412
41	H	-0.819	-1.2285	-1.4315	1.108377	-0.4095	7.061	-0.6423	-0.42304	0.466719
42	H	-2.3515	-3.52725	-0.43049	1.878097	-1.17575	9.0719	-3.0211	-0.55619	0.339223
43	H	0.0931	0.1397	-54.7755	0.373698	0.04655	8.5071	-2.4101	0.915612	0.719681
44	H	-0.2631	-0.39465	4.981756	0.628212	-0.13155	18.0034	-1.05	0.087284	-0.30064
45	H	-4.8476	-7.2714	2.656572	2.696553	-2.4238	19.427	-13.7104	0.620044	0.716374
46	H	-4.3741	-6.56115	-1.18925	2.561474	-2.18705	10.1821	-3.9602	-1.41071	0.149144
47	H	-2.0579	-3.08675	-0.13203	1.756943	-1.02895	7.8871	-2.9509	-0.44301	0.358991
48	H	-6.2299	-9.34475	-0.31261	3.056935	-3.11495	17.4823	-8.371	-0.70161	0.156021
49	H	-4.4909	-6.7363	1.106682	2.595448	-2.24545	20.0989	-9.2213	0.035763	-0.21859
50	H	-3.9496	-5.92435	-1.06697	2.434009	-1.9748	19.2237	-3.8173	-0.63699	-0.29
51	H	-0.2039	-0.3058	4.742521	0.553037	-0.10195	18.4619	-0.7893	0.062009	-0.21856

anticarcinogenic, anti-inflammatory, thermogenic, probitic, and antimicrobial properties in numerous human, animal, and in vitro studies[14-18].

The anticarcinogenic properties of green tea polyphenols, mainly EGCG, are likely a result of inhibition of tumor initiation and promotion, induction of apoptosis, and inhibition of cell replication rates, thus retarding the growth and development of neoplasms[19-22]. Green tea polyphenols antioxidant potential is directly related to the combination of aromatic rings and hydroxyl groups that make up their structure, and is a result of binding and neutralization of free radicals by the hydroxyl groups[23-27].

The potential health effects of catechins depend not only on the amount consumed but on their bioavailability which appears to be very variable. In order to known the catechin bioavailability and metabolism, it is necessary to evaluate their biological activity within target tissues[28-36].

Green tea is considered a dietary source of antioxidant nutrients: green tea is rich in polyphenols(catechins and gallic acid, particulary), but is also contains carotenoids, tocopherols, ascorbic acid (vitamin C), minerals such as Cr, Mn, Se or Zn, amd certain phytochemical compounds. These compounds could increase the green tea polyphenols (GTP) antioxidant potential. The antioxidant capacity of GTP has been assessed by several methods[37-41].

For example, Cao *et al*.[42] using the oxygen radical absorbance capacity (ORAC) assay found that green tea has a much higher antioxidant activity against peroxyl radicals than vegetables such as garlic, kale, spinach and Brussels sprouts. Langley-Evans [43]found that the total antioxidant capacity of green tea is more potent than that of black tea.Saffari and Sadrzadeh[44] investigated the antioxidant capacity of EGCG using erythrocyte membrane- bound[45-51].

ATPases as model, and the results indicated that EGCG is a powerful antioxidant that is capable of protecting erythrocyte membrane-bound ATPases against oxidative stress. Several

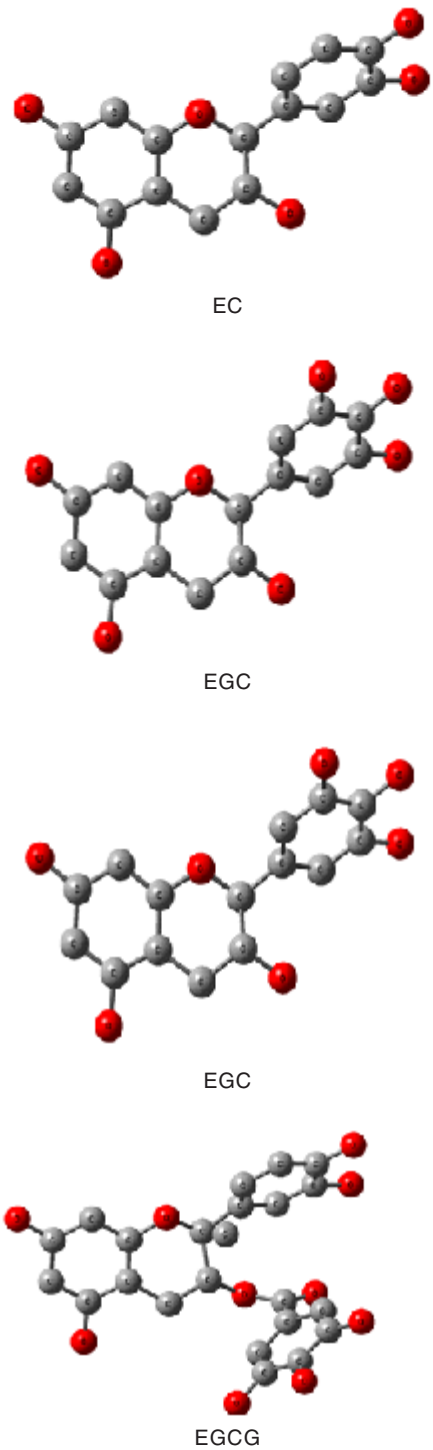

Fig. 1: Energetically favourable structure of four major catechins in green tea. EC, (-)-epicatechin; EGC, (-)-epigallocatechin; ECG, (-)-epicatechin-3-gallate; EGCG, (-)-epigallocatechin-3-gallate

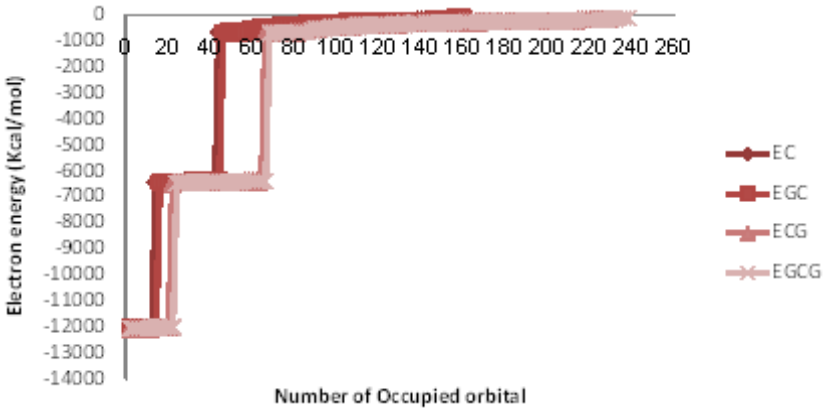

Fig. 2: Variation of electron energy in the occupied orbitals for EC, (-)-epicatechin; EGC, (-)-epigallocatechin; ECG, (-)-epicatechin-3-gallate; EGCG, (-)-epigallocatechin-3-gallate

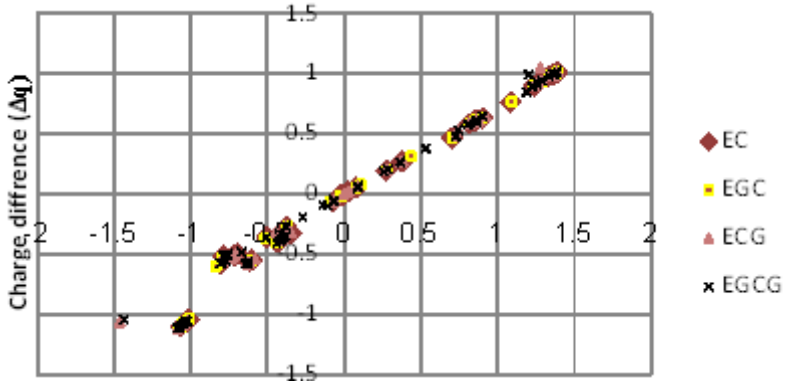

Fig. 3: Variation of charge difference (Δq) as function of bond moment for EC, (-)-epicatechin; EGC, (-)-epigallocatechin; ECG, (-)-epicatechin-3-gallate; EGCG, (-)-epigallocatechin-3-gallate

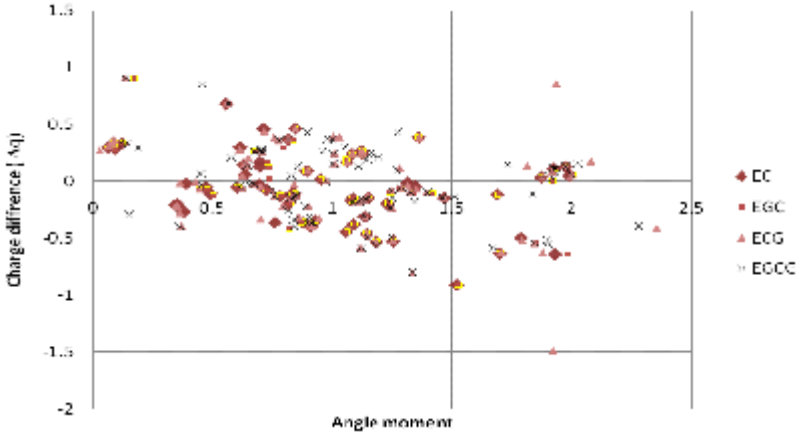

Fig. 4: Variation of charge difference (Δq) as function of angle moment for EC, (-)-epicatechin; EGC, (-)-epigallocatechin; ECG, (-)-epicatechin-3-gallate; EGCG, (-)-epigallocatechin-3-gallate

studies have shown that EGCG can act *in vitro*as an antioxidant by trapping proxyl radicals and inhibiting lipid peroxidation[44,52]. However, the antioxidant capacity of catechins determined *in vitro*is dependent upon the type of assay and it does not reflect factors such as bioavailability and metabolism[53-59].

Methods and Calculations

Computational methods are well placed to a theoretical approach that the first-principle calculation to obtain various aspects of drug properties of green tea molecules[60-63].

The first-principle quantum chemical calculations applied to investigation the nature of green tea molecules were performed in the density functional theory (DFT) system using the program package Gaussian 03. At first, the geometry of the molecules was optimized[64-66].

In the all calculations molecule were treated with 6-31G* basis set, carried out by B3LYP function[67,68].

All these cases have been taken into account for several parameters such as energy,dipole moment, quadrupole moment, energy gap, electron energy and etc[69-71].

As a result, energetically favourable structure of four molecules showed on figure 1.

NMR calculations also were performed and results were obtained according to output files data.NMR parameters were achieved by following equations:

$$\xi = \sigma_{ZZ} - I_{SO} \quad ...(1)$$

That *Iso*in equation (1) is Isotropic factor.

$$\Delta\sigma = \sigma_{ZZ} - \frac{1}{2}(\sigma_{XX} + \sigma_{YY}) \quad (2)$$

$$\eta = \frac{\sigma_{YY} - \sigma_{XX}}{\xi} \quad (3)$$

$$\sigma_v^{iso} = \sqrt{\frac{3}{2}}\xi \quad (4)$$

$$\sigma_{\pm} = \frac{1}{2}\xi \quad (5)$$

$$\Omega = \sigma_{33} - \sigma_{11} (6)$$

That Ω in equation (6) is Span factor.

$$S_{kew} = \sigma_{ZZ} - \sigma_{XX} (7)$$

$$K = \frac{3(Iso - \sigma_{YY})}{\Omega} (8)$$

That Δ_{YY}in equation (8) can be substitute with Δ_{22} for gaining other K factor [72,73].

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