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Nano Drug Delivery Study of Anticancer Properties on Ginger using QM/MM Methods

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ABSTRACT

Ginger is a one of the most important foods which as an anticancer drug. It is well-known for its ability to shrink tumors. The anti-cancer properties were observed in addition to ginger's role in reducing inflammation, as well as being a rich source of life-enhancing antioxidants. Ginger has long been used in traditional medicine as a cure for some diseases including inflammatory diseases[1].Ginger contains active phenolic compounds such as gingerol, paradol and shogaol that have antioxidant[2],anti-cancer[3], anti-inflammatory[4], anti-angiogenesis[5] and anti-artherosclerotic properties[6] (Fig.2). In the present work, we investigated the potential anti-inflammatory and anti-cancer effects of ginger extract including gingerol, andshogaol jointed to nanotubeas dug delivery technics. So, we have used Gussian 98 methods for calculation via (B3LYP-MP2-) with 6-31g*, basis sets .We has also studied NMR by changing the substituents in ginger for analyzing its properties.

Key words: Ginger, gingerol, paradol, shogaol, anti cancer, anti-inflammatory, anti artherosclerotic, antioxidants.

INTRODUCTION

Man's acquaintance with the medicinal properties of plants is of great antiquity. Even the higher mammals are said to be aware of the curative aspects of plant kingdom. Plants have been used in a number of systems of medicines in most countries. India is well known as the 'Emporium of Medicinal Plants'. The use of plants to treat various diseases in India dates back to the times of Rig-Veda (3500 to 1800 B.C.). Later, the monumental Ayurvedic works like Charaksamhita and Sushrutasamhita followed by other Ayurveda and Siddha treatises have incorporated nearly 700 plant drugs entering into several medicinal preparations used in the management of health care. In fact these systems have been in practice even in remote areas of our country for centuries1. Ginger consists of the fresh or dried roots of Zingiberofficinale. The English botanist William Roscoe (1753-1831) gave the plant the name Zingiberofficinale in an 1807 publication. The ginger family is a tropical group especially abundant in Indo-Malaysia, consisting of more 1200 plant species in 53 genera. The genus Zingiber includes about 85 species of aromatic herbs from East Asia and tropical Australia. The name of the genus, Zingiber, derives from a Sanskrit word denoting "horn-shaped," in reference to the protrusions on the rhizome 2, 3. Zingiberofficinalis Roscoe, commonly known as ginger belongs to family Zingiberaceae is cultivated commercially in India, China, South East Asia, West Indies, Mexico and other parts of the world. It is consumed worldwide as a spice and flavoring agent and is attributed to have many medicinal properties[1-6-7-10]**.**

The British Herbal Compendium reported its action as carminative, anti- emetic, spasmolytic, peripheral circulatory stimulant and antiinflammatory[4]. The oil of ginger is a mixture of constituents, consisting of monoterpenes (phellandrene, camphene, cineole, citral, and borneol) and sesquiterpenes (zingiberene, zingiberol, zingiberenol, ß-bisabolene, sesquiphellandrene, and others). Aldehydes and alcohols are also present 5, 6. A numeral of commercial variety of ginger exists. Nigerian Ginger is darker in color, minute size and more pungent taste. Cochin Ginger is habitually larger, well scraped, contains more starch and breaks with a shorter fracture. African Ginger is darker in color, more pungent in taste and less flavor than Jamaica Ginger. Ginger plant is propagated by rhizome cuttings each bearing a bud. The pieces of rhizome are planted in holes during March and April in a well- drained clayey soil. In December or January rhizomes are unruffled. Ginger requires a warm and humid atmosphere. A well distributed rainfall is required for its cultivation. If the area is getting fewer rainfalls, the crop needs habitual irrigation[7]**.**[1-11-15-17]

The major pungent compounds in ginger, from studies of the lipophilic rhizome extracts, have yielded potentially active gingerols, which can be converted to shogaols, zingerone, and paradol that have antioxidant anti-cancer), antiinflammatory, angiogenesis), and anti-atherosclerotic properties). Ginger has been known to comprise of the following nutrients: calcium, carbohydrate, dietary fiber, iron, magnesium,manganese,potassium,protein, selenium, sodium, and vitamin, C, E and B6. A fresh ginger contains 80.9% moisture, 2.3% protein, 0.9% fat, 1.2% minerals, 2.4% fiber and 12.3% carbohydrates .The composition varies with the type, varieties and agronomic condition and storage condition[4] consumption of fruits, vegetables, and whole grains may reduce cancer risk in some individuals. This association has been attributed to these foods being rich sources of numerous bioactive compounds (Milner,2004). Bioactive components present in fruits and vegetables can prevent carcinogenesis by blocking metabolic activation, by increasing detoxification, or by providing alternative targets for electrophilic metabolites (kuo *et al*., 2005). Numerous constituents of plant foods, including flavonoids (such as quercetin, rutin, and genistein), phenols (such as curcumin, epigallocatin-3-gallate and resveratrol), isothiocyanates, allyl sulfur compounds, indoles, and selenium have been found to be potent modulators of detoxification enzymes in vitro and in preclinical models (Milner ,2001 and Keum *et al*., 2004). The effect of plant extracts as antitumors was widely studied due to their low toxicity and side effect. The inhibition of ascites tumor cells by Nigella sativa seed extracts was investigated (Musa *et al*., 2004). Willow extracts antitumor activity which is due to the presence of Salicin (Zahran *et al*., 2005). Curcuma longa extracts and active constituents have a potential role in the prevention of cancer and the management of infectious and chronic diseases (Ahmad *et al*., 2008[2]**.**

Many herbs and spices are known to possess an array of biochemical and pharmacological activities in relation to its potential antiinflammatoryproperties; ginger extract has been shown to inhibit the activation of TNF-á and cyclooxygenase-2 expression during in vitro studies of human synoviocytes. Ginger extract possesses antioxidative characteristics, since it can scavenge superoxide anion and hydroxyl radicals.). Gingerol from ginger inhibit, at high concentrations, ascorbate / ferrous complex induced lipid peroxidation in rat liver microsomes[4]**.**

Tumor promotion is closely linked to inflammation and oxidative stress; so compounds that exhibit anti-inflammatory and/or antioxidant properties could acts as anticarcinogenic agent (Masuda *et al*., 2004).Some phenolic substances present in ginger(Zingiberofficinale Roscoe, Zingiberaceae), generally, possess strong antiinflammatory, anti-oxidative and anti-mitotic properties and exert substantial anti-carcinogenic and anti-mutagenic activities (Surh, 2002 ; Bode, 2003; Kim *et al*.,2005a ; Vijayapadma *et al*., 2007 and Choudhury *et al*., 2010)[2].

In Saudi Medical Journal, the authors report that both triglycerides and total cholesterol decreased significantly from baseline in the treatment compared with the placebo group. LDL cholesterol was reduced and HDL cholesterol was increased in the treatment group compared with placebo, but these changes were not significant. Furthermore, ginger acts as a hypolipidemic agent in cholesterol-fed rabbits Feeding rats with ginger significantly elevated the activity of hepatic cholesterol-7a-hydroxylase, the rate-limiting enzyme in bile acids biosynthesis, thereby stimulating cholesterol conversion to bile acids, resulting in elimination of cholesterol from the body[3] (According to one study oral administration of 170mg/kg zingerone may reduce the body weight, blood glucose level and prevent the fat storage through increasing norepinephrin-induced lipolysis in adipocytes. There was also distinct decrease in lipid per oxidation and enhancement of fibrinolytic activity in ginger treated animals. Authors suggested the protection was probably because of its free radical scavanging, prostaglandin inhibitory and fibri properties. Tea is also reported to have multiple pharmacological actions and improved health related quality of life . It acts both as primary as well as secondary antioxidant by sequestration of metallic ion and by scavenging active oxygen species. Several epidemiological studies have demonstrated an inverse relationship between tea consumption and cholesterol. The tea catechin contains Epigallocatechingallate (EGCG) and EGC which were found to inhibit intestinal glucose transporter SGLTI,

Including its effect on controlling blood sugar.Ingestion of extract of tea in rats has significantly decreased plasma cholesterol and triglyceride concentrations and the ratio of low and very low density lipoprotein cholesterol concentrations to high density lipoprotein cholesterol concentrations. Tea polyphenols also increase fecal excretion of total lipids and cholesterol in rodents . One study demonstrated that the addition of five servings of tea per day to an NCEP Step I-type diet appreciably reduces total and LDL cholesterol in mildly hypercholesterolemic volunteers. Tea extracts were found to exert rapid normalization of blood glucose levels within three weeks on streptozotocin induced Diabetes in rats . Ginger and Tea both has been studied extensively in animal and in vitro models separately, however, their potential effects in combination have not yet been studied in humans. Since both Tea and Ginger are involved in lowering the lipid profile, these together can be used to see the cumulative effect on lipid profile, glucose level and insulin resistance[3].

In addition chemotherapy with plant-derived compounds or dietary phytochemicals has emerged as an accessible and promising approach to cancer control and management (Surh, 2003). A growing trend among some cancer patients is to combine conventional therapy with some form of complementary therapy (Vapiwala *et al*., 2006). These diverse pharmacological activities of their major principles have already been confirmed (Surh *et al*., 2002). Several lines of evidence suggest that 6-gingerol is effective in the

Table 1:

Molecule	E HF Kcal/mol	Dipol Totally	Dipol Totally calculated	Gap ENERGY Kcal/mol	Determinan Distance Matrix
a	-648531.4978			-115.5121746	-1.27621E+15
b	-439321.3073	3.1220		-117.8140363	- 2306040772
c	-597129.262969661	3.7202		-95.5942	-3.5031E+14

Table2:

Isotropic	ξ	ΩSpan	Δσ	η	σ^{iso}_{u}	σ^{+}_{-}	Skew	K	K
a)variation of NMR factor in eackhatm on molecule									
81.4199	72.421	162.1783	108.6315	-0.7189	10.42264362	36.2105	82.5997	1.15136612	0.282648
52.0383	61.9393	139.5543	92.9089	0.149178	9.638928882	30.96965	97.5289	0.56643758	0.400324
51.9336	61.3652	127.1564	92.0478	0.176889	9.59415447	30.6826	97.4752	0.595845746	0.396107
85.9575	69.9662	158.45	104.9494	-0.82796	10.24447656	34.9831	75.9847	1.210750394	0.16935
63.973	88.348	190.3553	132.522	0.371764	11.51182001	44.174	148.9443	0.437366861	0.483797
73.8344	85.0643	183.8658	127.5964	0.596659	11.29585986	42.53215	152.9736	0.279903604	0.08337
242.2039	51.0124	111.5965	76.5186	-0.33479	8.747491069	25.5062	67.9794	0.915227628	0.284073
157.2955	-12.19	37.6756	-18.2851	0.964848	4.276096	-6.095	-24.1658	-0.017064095	0.367185
139.3559	-27.5274	75.4493	-41.2911	0.875858	1.22474	-13.7637	-53.3461	-0.067937012	0.583576
-9.0496	-52.1006	193.1892	-78.151	-1.44116	8.840299	-26.0503	-40.6084	-0.987522594	0.672309
138.437	-6.0415	26.72	-9.06225	0.686138	1.22474	-3.02075	-11.1349	-0.106448353	0.008757
118.1012	-11.6463	44.8582	-17.4696	-0.18498	24.179647	-5.82315	-16.3924	-0.461480844	0.212249
154.0904	-3.5746	31.1057	-5.3619	2.628042	2.315577	-1.7873	-10.059	0.280636668	0.206576
159.1341	1.4868	36.9604	2.2302	-10.1656	1.493385416	0.7434	-5.3269	0.673734592	-0.11455
155.7628	-2.4792	39.7945	-3.7188	5.547596	1.928419	-1.2396	-10.5956	0.4249733	0.268809
163.2984	-1.5462	26.1199	-2.3193	5.850601	1.522292	-0.7731	-6.8424	0.43070609	0.177095
173.3987	2.4389	27.0837	3.65835	-3.19123	1.912681364	1.21945	-0.2332	0.566133874	0.603518
-286.682	-531.016	1206.708	-796.524	-0.60344	28.22275	-265.5081	-636.306	-1.058400292	0.213568
267.3473	31.2893	84.4222	46.934	-0.53182	6.850835715	15.64465	38.6138	0.851608937	0.903736
264.2121	39.7657	129.3409	59.64865	-2.36492	7.723247374	19.88285	12.6273	1.551813077	-0.62046
137.4482	-14.3545	71.581	-21.5318	-4.28037	4.64023	-7.17725	9.1895	-1.588351658	0.734097
25.5994	-3.4573	7.2917	-5.1859	0.789402	2.27726	-1.72865	-6.5505	-0.149759315	-0.23735
26.111	-3.9474	11.2322	-5.9211	2.280032	2.43333	-1.9737	-10.4212	0.67477431	0.566763
25.5578	-3.637	8.5746	-5.45545	-0.67861	2.335701	-1.8185	-4.2214	-1.067979847	0.197152
27.3937	-9.5285	19.681	-14.2927	0.104487	3.78057	-4.76425	-14.7905	-0.650332808	-0.37551
29.5121	-1.1848	7.3718	-1.77725	1.091914	1.33311	-0.5924	-2.4241	0.022138419	-0.09299
29.6091	-0.3811	8.548	-0.5717	7.054841	0.756075	-0.19055	-1.916	0.404901731	-0.51482

29.8298	-1.8788	9.1691	-2.81825	1.884448	1.678749	-0.9394	-4.5885	0.271826024	-0.2859
29.0288	-1.6335	11.9246	-2.4502	3.514172	1.565324	-0.81675	-5.3204	0.516621103	0.512143
30.1752	-2.1855	5.9302	-3.2782	-2.1908	1.8105938	-1.09275	-0.8842	-1.763869684	0.671563
29.8026	-1.8846	5.2134	-2.82695	0.584899	1.681338	-0.9423	-3.3781	-0.225112211	-0.63166
28.2076	-1.2263	5.0425	-1.8395	0.128517	1.35626	-0.61315	-1.9183	-0.317937531	0.650987
30.7124	-1.7355	8.7383	-2.60325	0.284587	1.613459	-0.86775	-2.8502	-0.2131307	-0.70242
30.5879	-0.7326	9.6518	-1.0989	9.002457	1.0482843	-0.3663	-4.3965	0.911115025	-0.08995
30.1533	-1.815	9.1304	-2.72255	0.872782	1.65	-0.9075	-3.5146	-0.037950145	-0.71428
30.9523	-0.2333	8.4668	-0.3499	17.14702	0.5915657	-0.11665	-2.3501	0.667406812	-0.47763
30.7616	-1.0936	7.6989	-1.64045	0.012162	1.280781	-0.5468	-1.6471	-0.210497604	-0.65394
30.7654	-0.2236	7.5918	-0.33535	14.91905	0.5791372	-0.1118	-2.0033	0.614952976	-0.8434
30.6812	-0.5782	8.884	-0.8673	-4.39018	0.931289	-0.2891	0.4019	-0.526215669	-0.30925
30.7308	0.5433	9.1134	0.81495	-8.44892	0.902745811	0.27165	-1.4802	0.844953585	-0.24811
31.0649	-2.4414	11.0439	-3.66205	1.529327	1.91366	-1.2207	-5.5289	0.175535816	0.662185
31.2299	-0.1281	9.0574	-0.1921	11.17721	1.224744	-0.06405	-0.908	0.215922892	0.477985
31.2119	0.9	8.9365	1.35005	1.579889	1.161895004	0.45	2.061	-0.087584625	0.401097
31.8457	6.6993	16.6556	10.049	-0.21444	3.170007886	3.34965	9.3307	0.73272653	0.711022
28.3217	-4.0965	10.1473	-6.14485	0.208544	2.47886	-2.04825	-6.572	-0.479299912	0.347235
28.626	-3.1875	8.9815	-4.7812	-1.9626	2.1866069	-1.59375	-1.6533	-1.577108501	0.507009
28.6018	0.975	9.1232	1.4625	1.907282	1.209338662	0.4875	2.3923	-0.145442389	0.579829
b)variation of NMR factor in eackhatm on moleculeb									
81.4375	81.5031	162.0291	122.2546	-0.55738	11.05688247	40.75155	99.5403	1.175082	0.289598
51.8988	70.4471	140.0636	105.67065	0.358108	10.27962305	35.22355	118.2845	0.484274	0.401755
51.816	66.7597	127.8851	100.1395	-0.37172	10.00697507	33.37985	87.7316	1.074113	0.399351
86.0403	79.1818	158.9326	118.77265	-0.61341	10.89828886	39.5909	94.4873	1.205722	0.184961
64.312	98.129	190.2653	147.19345	0.390968	12.13233283	49.0645	166.3761	0.47116	0.474014
74.1077	88.371	183.1839	132.55645	-0.16529	11.51331837	44.1855	125.2531	0.843231	0.070287
241.8254	56.4411	112.7148	84.6616	-0.76728	9.201176555	28.22055	63.0085	1.327428	0.286836
157.3573	-13.3667	37.3482	-20.05005	1.643704	4.4777	-6.68335	-31.0355	0.345567	0.394878
143.0239	-21.3095	67.8569	-31.96425	2.312701	5.653693	-10.65475	-56.6055	0.618353	0.694912
-5.9463	-45.9353	188.8939	-68.90295	-3.65105	8.30078	-22.96765	14.9532	-1.69657	0.640915

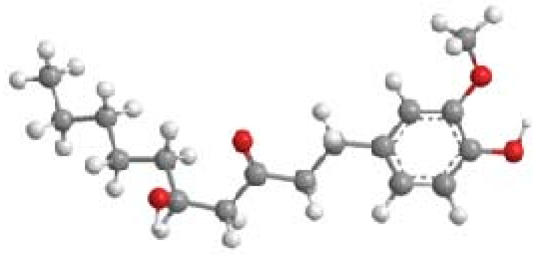
-288.135	1067.47	-490.176	821.8697	0.658569	40.01505592	533.7349	1173.371	3.654413	-0.52692
161.5458	1.0105	52.1097	1.51575	-32.8999	1.231157991	0.50525	-15.1069	0.986068	0.885428
263.5932	47.2119	128.7875	70.8179	-1.24449	8.415334218	23.60595	41.4406	1.234203	-0.62084
137.3064	-17.0405	71.682	-25.56085	-3.85149	5.05576	-8.52025	7.2548	-1.72997	0.734975
25.6107	-3.5056	6.9737	-5.25835	0.316551	2.29312	-1.7528	-5.8132	-0.51532	-0.2804
26.0557	-4.1198	10.9763	-6.1797	1.435798	2.4859	-2.0599	-9.1373	0.245356	0.539772
25.6319	-3.6092	8.2041	-5.41385	0.017317	2.32675	-1.8046	-5.4451	-0.64848	0.197791
27.3699	-10.1976	19.563	-15.29635	-0.46708	3.91106	-5.0988	-12.9148	-1.14711	-0.36778
29.5045	-1.0685	8.3413	-1.6027	1.103978	1.26599	-0.53425	-2.1925	0.019997	-0.36631
29.6369	-0.6857	8.1072	-1.0285	0.570512	1.014174	-0.34285	-1.2241	-0.05447	-0.11005
29.6513	-0.8601	9.1773	-1.29005	2.273108	1.1358477	-0.43005	-2.2676	0.179007	0.013926
29.7979	-0.4947	8.7571	-0.74205	5.618961	0.861423	-0.24735	-2.1319	0.391397	-0.14066
30.18	-1.7169	6.2387	-2.57525	-0.16256	1.604789	-0.85845	-2.4357	-0.47986	-0.03895
30.4957	-1.679	7.6851	-2.51845	3.915724	1.586978	-0.8395	-5.8057	0.955537	0.651833
30.1477	0.2036	5.8719	0.3055	-9.8556	0.552630075	0.1018	-0.6978	0.564655	-0.37506
28.3259	-4.2312	10.0165	-6.34675	-1.06289	2.51928	-2.1156	-4.0981	-1.3071	0.347427
28.617	-0.0747	9.0415	-0.112	-54.6212	0.334738	-0.03735	1.9281	-0.68929	0.628469
28.6127	-2.4119		-3.6178	-1.6101	1.902064	-1.20595	-1.6761	-1.05458	0.563373
c)variation of NMR factor in eackhatm on molecule c									
81.4946	-80.83075	161.7759	95.77145	0.856855838	11.01118	-40.415375	61.1413	-9.80979	-2.2806
51.9666	-47.03145	139.89	73.48835	0.043100946	8.39923	-23.515725	72.4748	3.731634	2.723042
51.9091	-57.73155	127.7605	69.56395	0.585075232	9.30576	-28.865775	52.6753	156.9174	66.03446
86.0402	-80.75845	159.6024	98.81015	0.868063961	11.00625	-40.379225	63.7584	-9.15391	-1.32279
63.8776	-66.4995	190.3892	99.6091	-0.073236641	9.987454	-33.24975	102.0442	2.41845	2.422065
74.0947	-49.6849	182.7778	86.1006	0.36142973	8.632922	-24.84245	77.1218	37.34168	4.21879
242.2413	134.45425	112.0174	61.52685	-0.383048509	14.20145679	67.227125	35.7756	-0.67217	-0.15462
157.372	167.29645	37.5174	-12.41395	-0.079230014	15.84123338	83.648225	-19.0414	-0.04234	-0.07535
140.7702	160.3913	64.6209	-34.7428	-0.332968185	15.51086555	80.19565	-61.4454	-0.22434	-0.25551
3.0407	134.38385	183.1866	-40.59525	1.149187942	14.19773838	67.191925	36.6209	-8.10727	2.734415
69.1439	241.01245	157.4016	-115.60075	0.147164597	19.01364444	120.506225	-97.8665	1.010736	0.454533
48.6621	276.1374	220.7375	-128.6773	0.404911468	20.35205395	138.0687	-72.7717	2.440787	-0.40073
153.6438	150.67575	33.7781	-3.99365	-0.110076771	15.03374953	75.337875	-12.2866	-0.12587	0.002999

157.5241	159.1476	35.3611	-10.4085	-0.154001694	15.45061164	79.5738	-22.663	-0.14626	-0.05538
155.1278	160.6066	39.658	-13.2846	-0.152347413	15.5212725	80.3033	-25.5186	-0.12963	-0.06235
163.41	166.369	25.6546	-7.4599	-0.084000024	15.79726242	83.1845	-14.4474	-0.07592	-0.02217
173.643	169.66315	26.5482	-4.18405	-0.112676795	15.9528908	84.831575	-13.7426	-0.1307	-0.0869
-225.996	961.1492	-353.487	-672.5195	0.604385875	37.97003819	480.5746	-382.067	9.892146	-1.89347
263.6677	136.411	127.382	65.4635	-0.586052444	14.30442239	68.2055	25.4915	-0.77833	0.340067
137.2971	210.315	71.5101	-29.4402	0.321083137	17.76154554	105.1575	4.3241	0.983155	-0.39595
25.6318	29.87195	6.9931	-3.41135	-0.020644785	6.693872198	14.935975	-3.7197	0.084711	0.067407
26.0429	28.44785	11.1777	-3.90625	-0.19708695	6.532363661	14.223925	-6.7096	-0.13751	-0.18887
25.6344	32.11515	8.3599	-4.42525	0.036148049	6.94065739	16.057575	-3.8448	0.209181	-0.05717
27.3856	45.0794	19.6044	-11.0474	0.13149687	8.223083363	22.5397	-8.0835	0.562157	0.206182
29.5205	26.05125	8.2594	2.23055	-0.038013531	6.251149894	13.025625	1.7354	-0.13374	0.066964
29.57	33.49955	8.1202	-2.79795	0.011877771	7.088675828	16.749775	-2.599	0.10553	0.113485
29.7789	28.2988	8.8734	-0.9807	-0.197018955	6.515228315	14.1494	-3.7684	-0.22006	0.042138
29.7302	33.9856	8.8305	-4.3404	-0.090144061	7.139915966	16.9928	-5.8722	-0.00716	0.006573
26.3163	31.9077	11.9085	-7.2948	-0.259185087	6.918204247	15.95385	-11.4298	-0.13538	-0.13081
24.9555	27.7534	7.7796	-4.3442	-0.215786174	6.45213918	13.8767	-7.3386	-0.14365	-0.13952
30.1109	22.8654	8.0243	2.8813	-0.297724947	5.856457974	11.4327	-0.5225	-0.4274	0.08291
29.9177	38.4835	7.3581	-5.3069	0.077430587	7.597713472	19.24175	-3.817	0.289811	0.028644
30.5463	21.6421	8.2178	4.9215	-0.216448496	5.69764425	10.82105	2.5793	-0.42722	0.138742
30.8344	39.62045	7.5288	-6.48395	0.007104917	7.709129328	19.810225	-6.3432	0.185765	0.13045
30.7428	22.61125	7.5624	4.15975	-0.228660512	5.823819623	11.305625	1.5746	-0.40851	0.170477
30.7598	39.18145	7.3147	-5.98395	0.022615294	7.666301259	19.590725	-5.5409	0.201459	0.106634
30.6745	20.40095	9.0923	5.72435	-0.258914413	5.531855475	10.200475	3.0833	-0.49464	0.076666
30.6922	40.6511	8.785	-6.2621	0.079181129	7.808754702	20.32555	-4.6527	0.313777	0.066604
31.0372	34.125	10.905	-4.3636	-0.160023443	7.154544011	17.0625	-7.094	-0.10037	-0.18617
31.2589	22.16675	9.0674	6.01805	-0.096365051	5.766292136	11.083375	4.95	-0.35054	-0.15525
31.2469	37.69405	9.0372	-5.00715	-0.012153112	7.519379961	18.847025	-5.2362	0.118411	-0.12339
28.3416	36.4431	10.0408	-4.557	0.111159589	7.393554625	18.22155	-2.5315	0.344426	-0.11159
28.6315	33.0649	8.9443	-2.3777	0.076401259	7.042538605	16.53245	-1.1146	0.207325	-0.16248
28.6141	34.44255	9.0065	-2.20005	0.168108923	7.187755213	17.221275	0.695	0.389884	-0.19272

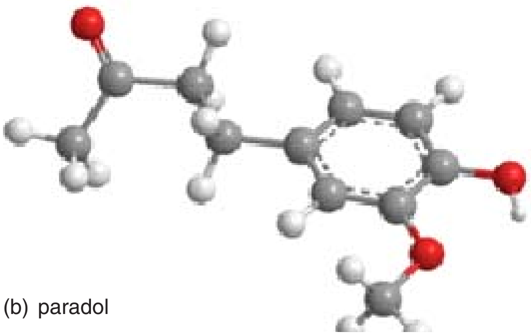
suppression of the transformation, hyperproliferation, and inflammatory processes that initiate and promote carcinogenesis, as well as the later steps of carcinogenesis, the angiogenesis and metastasis (Suzuki *et al*., 1997; Bode *et al*., 2001; Kim *et al*., 2005a: 2005b; Lee *et al*., 2008). It is regarded as a promising chemopreventive dietary agent exhibiting inhibition of cyclooxygenase and lipoxygenase activities (Kiuchi *et al*., 1982: 1992; Huang *et al*., 1991), apoptosis induction (Lee *et al*., 1998; Chauhan, 2002), and anti-tumorigenic effects (Park *et al*., 1998; Surh *et al*., 1999). The pungent vallinoids of ginger, [6]-gingerol and [6]-paradol, exhibit antiproliferation activity in liver, pancreatic, prostate, gastric, and leukemia cancer cells (Lee *et al*., 1998; Chen *et al*., 2007; Shukla and Singh, 2007). Furthermore, [6]-shogaol has also been shown to exhibit anticancer activities against breast cancer, anti-proliferation activity (through disruption of microtubule network of non-small lung epithelium cancer) (Choudhury *et al*., 2010), and anti-invasion on human hepatocellular cell (Weng *et al*. 2010**).** With this motivationwe start this present study.

EXPERIMENTAL

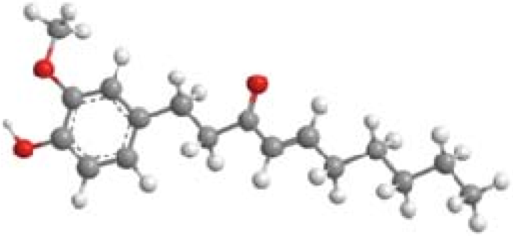
As with all the previous in this study first time we have prepared 3 molecule gingerol, paradol and shogaolin gussview.



(a)gingerol



(b) paradol



(c)shogaol

Fig. 1: (a) Ginger Plant with Flower ;(b)Fresh ginger rhizome

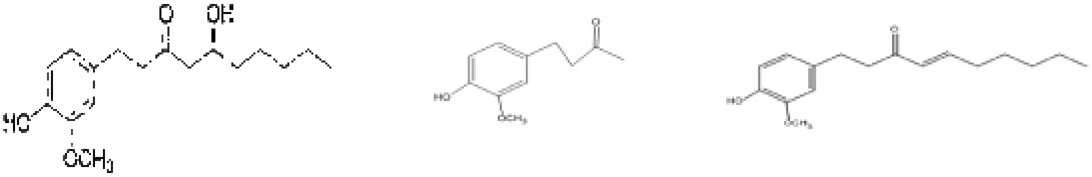
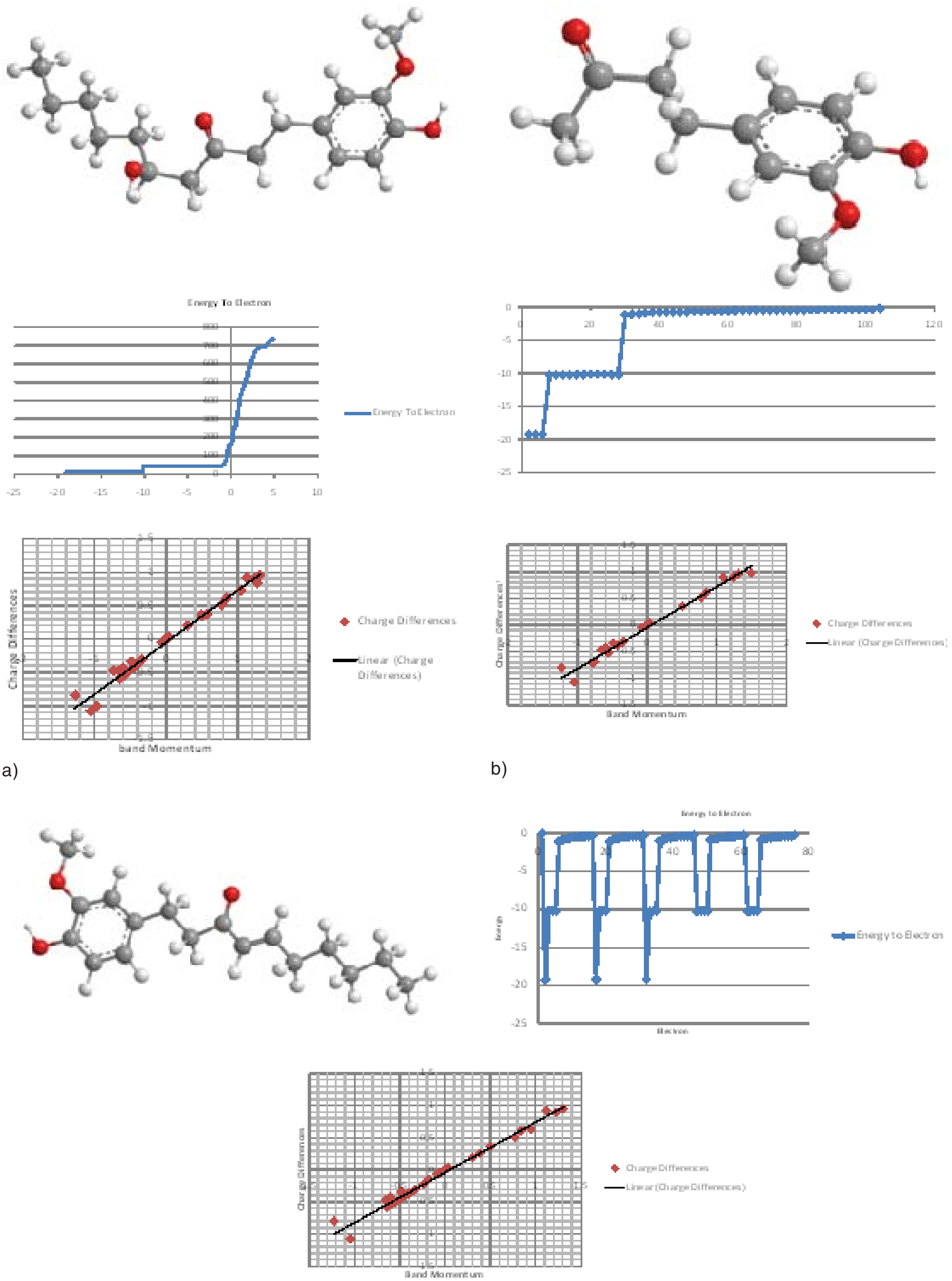


Fig. 2. Active phenolic compounds of Ginger such as (a)gingerol ;(b) paradol and (c)shogaol.



c)

Fig 3. : Variation of charge differences as function of band moumentumand variation energy to electron

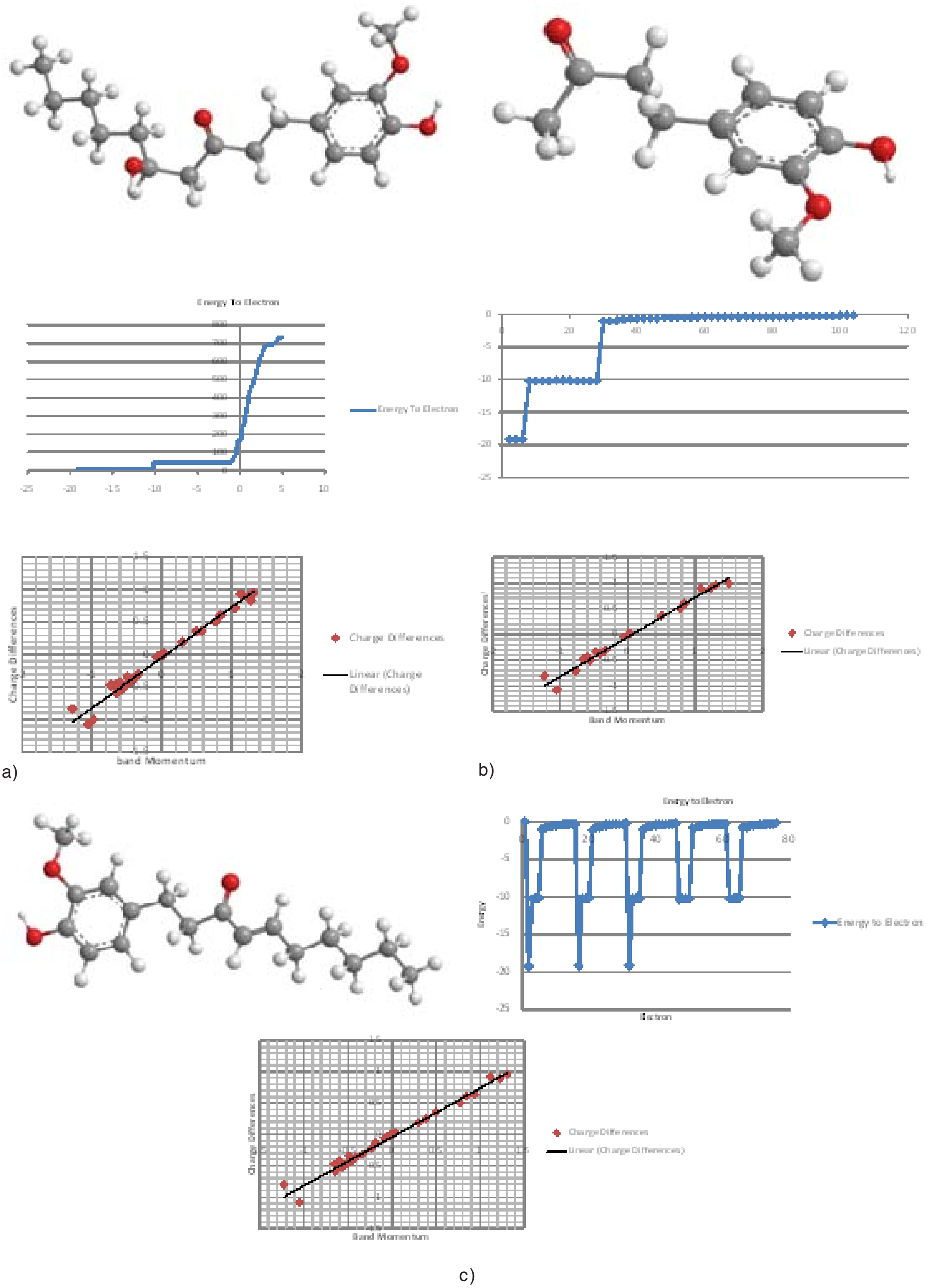
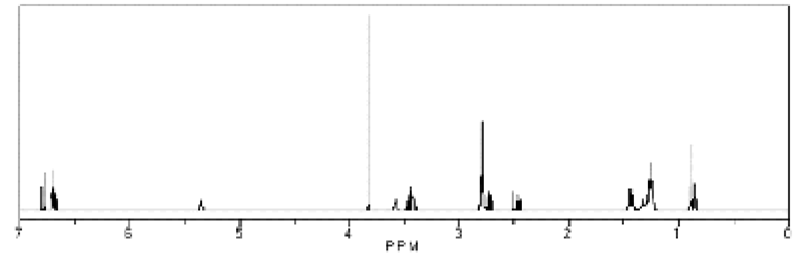
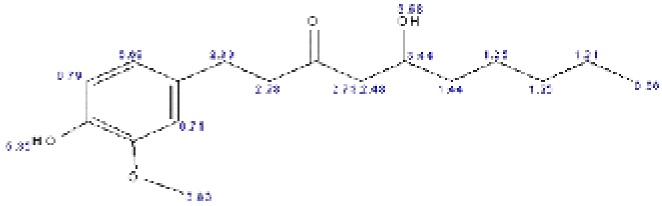
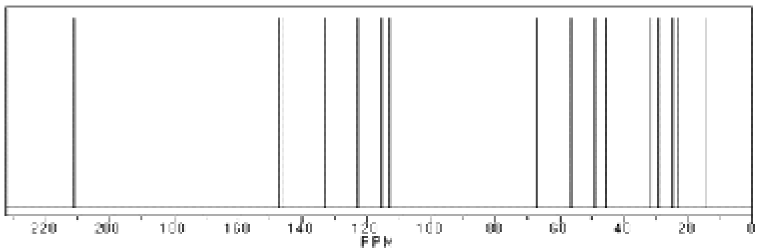
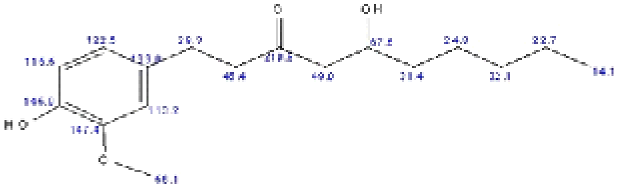


Fig. 4: H NMR and C NMR a,b,c Molecules

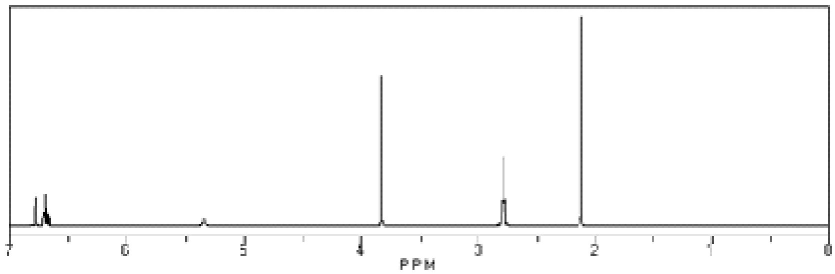


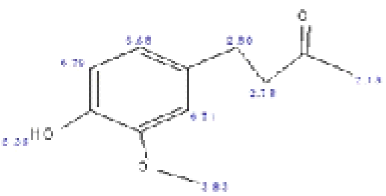


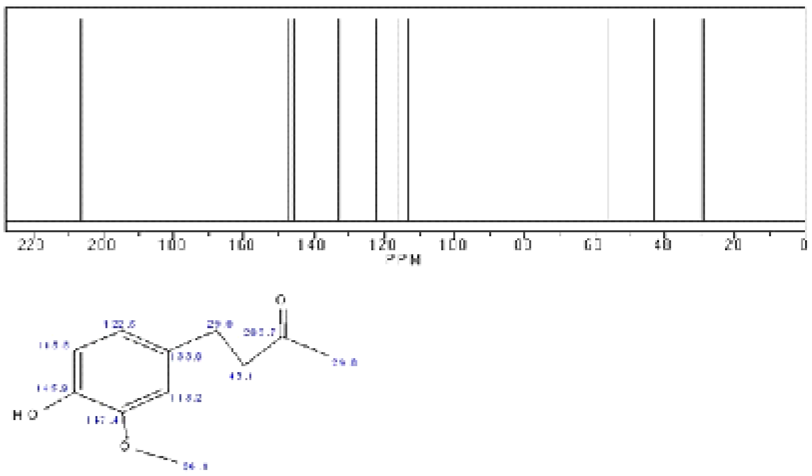




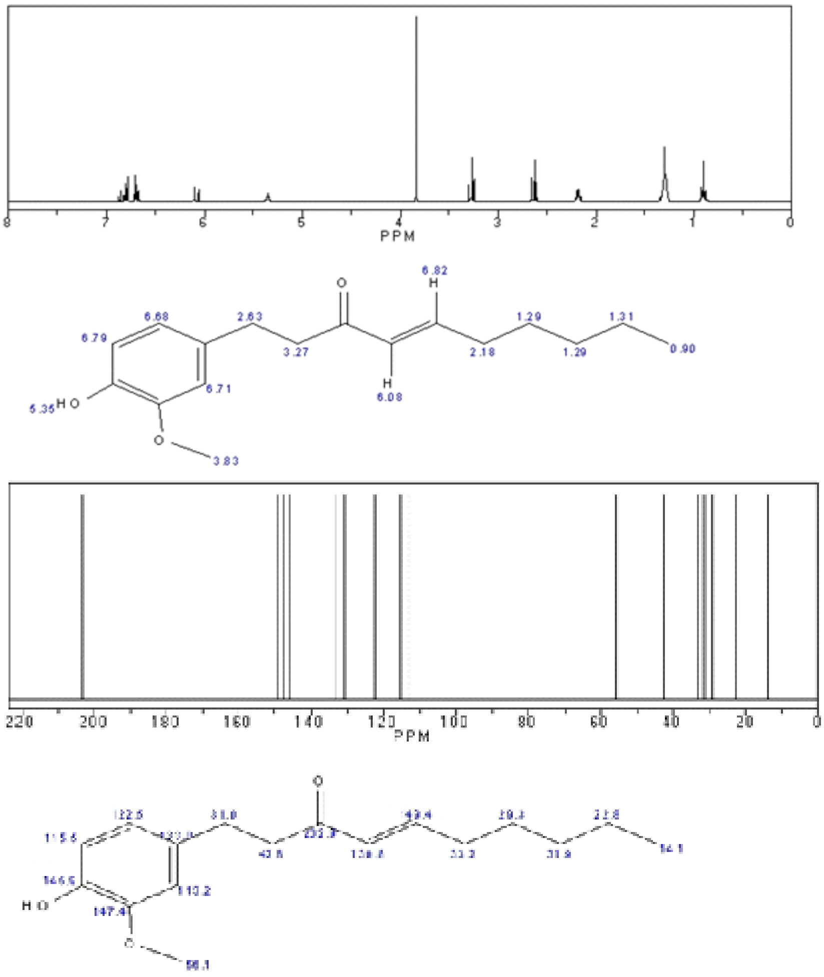
a)






PPM
HO

b)


8
7
6
5
4
3
2
1
0
PPM
6.82
H
6.68
2.63
1.29
1.31
6.79
3.27
2.18
1.29
0.90
H
6.08
6.71
5.35 HO
3.83
220
200
180
160
140
120
100
80
60
40
20
0
PPM
HO

c)

Fig. 6

We have also emploied an ab initio method to study, check and discussion.

Then, we consider 3 molecular of ginger family and study its behavior using ab initio calculations within Gussian 98 methods for calculation via the (B3LYP-MP2-) with 6-31g*, basis sets. We compare the Gap Energy (E HF), Dipol Totally ,DET distance matrix values obtained from the present first principles total energy calculations

. Here, we further investigated the roles of Number of atoms , The number of functional groups present in the substitution of, Types of bonds between two atoms, Increased or decreased by the factor ring resonator , (5):The chemical shifts and the factors NMR.by determin all All existing parameters.

In facct ,we calculate NMR factors and then compare data and We draw diagrams associated with them According to Fig 4.

RESULTS AND DISCUSSION

We first consider each molecule with Gussian09 and preoared opt each molculeAs shown in figure 1.Infact in table you observe data for all 3 molecule.

We obtained data NMR molecules according with figure 2. In Table a, b and c we list various

Parameters and calculated values relevant for the calculations of data NMRand fig 5 shown H NMR and C NMR. It can be seen variation of charge differences as function of band moumentum and variation energy to electron in the graphs in Fig. 3

Shown in table 1. There are a variety of E HF,GapEnergy,Totallydipol,det Distance Matrix, which we can exclude as the reason for the observed (1): Number of atoms :(2) The number of functional groups present in the substitution of, (3): Types of bonds between two atoms, (4): Increased or decreased by the factor ring resonator, (5):The chemical shifts and the factors NMR.As above, these effects ,which substituted or have a number of different atoms, can exacerbate in other models of molecules ginger. **All** This may have direct effects on the antioxidant anti-cancer anti-inflammatory, anti-angiogenesis and anti-artherosclerotic properties

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