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ORIENTAL JOURNAL OF CHEMISTRY
An International Open Free Access, Peer Reviewed Research Journal

www.orientjchem.org

ISSN: 0970-020 X
CODEN: OJCHEG
2014, Vol. 30, No. (4):
Pg. 1703-1718

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

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http://dx.doi.org/10.13005/ojc/300430

(Received: September 28, 2014; Accepted: November 03, 2014)

ABSTRACT

Nano-biotechnology takes most of its fundamentals from nanotechnology which most of the equipment designed for nano-biotechnological are based on other existing nanotechnologies. Nano-biotechnology is often used to describe the overlapping multidisciplinary activities associated with chemistry, biology and nano-medicine. In this investigation, the ab initio calculations were implemented using Gaussian program package based on density functional level of theory (DFT) to achieve the drug delivery technic for unraveling of linkage of Jackfruit to single walled carbon nanotubes. NMR investigation gives deeper physical insight into the impact of different structures. In this work NMR parameters were calculated at the Ethyl isovalerate, Propylisovalerate, Isobutyl isovalerate and 3-methyl butyl acetate extracted of Jackfruit with different functional groups in their active sites so, the anticancer properties of this compound have been clarified.

Key words: Jackfruit, CNT, anticancer, NMR, DFT, effective compounds

INTRODUCTION

The Jackfruit belongs to the Mulberry family that is native to parts of Southern and Southeast Asia. It can also be found in East African and Brazil. The fruit is the largest tree-borne fruit in the world. The Jackfruit is has an abundance of vitamin C which helps to protect against viral and bacterial infection[1-5]. It helps in strengthening the immune system as it support white blood cell function. Vitamin C is widely known for its ability to prevent colds and flu. Being rich in phytonutrients like Lignans, Isoflavines and Saponins that are all known for their anti-cancer and anti-aging properties, the Jackfruit helps in destroying cancer-causing free radicals and slows down the degeneration of cells that leads to degenerative diseases. These phytonutrients protect the skin and help to keep it supple and smooth. The potassium in the Jackfruit is found to help in lowering blood pressure and reverses the effects of sodium that causes a rise in blood pressure that affects the heart and blood vessels[6-10]. This helps in preventing heart disease and strokes. Potassium also helps in

preventing bone loss and improves muscle and nerve function. Another heart friendly property found in the Jackfruit is due to vitamin B6 that helps reduce homocysteine levels in the blood thus lowering the risk of heart disease. The high fiber content of Jackfruit prevents constipation as it bulks up food consumed which then passes more easily through the gut[11-16.] The fiber also offers protection against colon mucus membrane by mopping up carcinogenic chemicals in the large intestine and preventing colon cancer. The anti-ulcer properties help cure ulcers and other digestive disorders[17-20]. Certain extracts from the root of the Jackfruit plant are said to help cure diarrhea and found to be beneficial for those suffering from asthma. With a small amount of Vitamin A available, it helps maintain good vision and smooth skin. Vitamin A is instrumental in preventing age related macular degeneration and night blindness. The Jackfruit contains iron that helps prevent anemia and aids in proper circulation, magnesium that is important in the absorption of calcium. Calcium is important in the development strong teeth and bones and helps prevent bone related disorders like osteoporosis. It has copper that helps maintain a healthy thyroid and plays an important part in hormone production and absorption[21-24]. The calcium contained in the fruit also helps in the clotting of blood. With a large amount of simple sugars like fructose and sucrose, it boosts energy and as it contains no fat or cholesterol, it is perfect as a diet food. This exotic fruit is a great fruit and can be served raw or cooked but either way it has many health benefits[25,26].

Biopolymers are polymers which are produced from renewable natural sources, are often biodegradable, and not toxic to generate[27,28]. They offer the benefits of being bio-degradable, non-toxic and ability to bind with a number of drugs. They can be manufactures into a number of pharmaceutical compounds and hence be used as novel drug delivery carriers. Jackfruitcontains morin, carotenoids, provitaminA[29-32]. It is used medicinally asa laxative, tonic and demulcent. In more recent years many drugs have been shown to achieve a better systemic bioavailability by self medication through the oromucosal route than by oral administration[33-38].

It is now widely accepted that the beneficial effects of fruits and vegetables for the prevention of certain diseases are due to the bioactive compounds they contain[39-42].

Recent years have seen increased interest on the part of consumers, researchers, and the food industries into how food products can help maintain health; and the role that diet plays in the prevention and treatment of many illnesses has become widely accepted . The aim of this review was to present an overview of the functional, medicinal, and physiological properties of the Jackfruit[43 -45].

Drug delivery is a rapidly growing area that is now taking advantage of nanotube technology. These nanotubes function with a larger inner volume to be used as the drug container, large aspect ratios for numerous functionalization attachments, and the ability to be readily taken up by the cell[46-50].

In this work, we have used computational chemistry techniques to investigate current problems in biology, medicinal chemistry and materials research. The group also develops novel methods for predicting biological activity and molecular properties based on quantum mechanics (QM) methods. Due to this purpose ,we have studied the chemical properties of effective structures in Jackfruit consisting of Ethyl isovalerate ,Propyl isovalerate ,Isobutyl isovalerate and 3-methyl butyl acetate using theoretical and computational methods[51-54].

Computational Methods

In this study, we have investigated various properties of effective compounds of Jackfruit extract. This molecule has effective role in anticancer characteristic of Jackfruit. Ab-initio calculations were carried out by density functional theory method (DFT). This showed the significant role of different atoms of mentioned compound on anti-cancer characteristics of Jackfruit.

The chemical shift refers to phenomenon which associated with the secondary magnetic field created by the induced motions of the electrons that surrounding the nuclei when in the presence of an applied magnetic field[55-57]. The shielding Δ, is the differential resonance shift due to the induced motion of the electrons. The chemical shielding

tensor is commonly referred to the chemical shift anisotropy (CSA) tensor according to the possession of second rank properties. The CSA tensor can be described by three additional parameters [58].

a) The isotropic value (σ_{iso}), of the shielding tensor which can be defined as:[59-61].

$$\sigma_{iso} = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33})$$

b) The chemical shift anisotropy parameter ("Ã), due to the following expression:

$$\text{if} |\sigma_{11} - \sigma_{iso}| \geq |\sigma_{33} - \sigma_{iso}| \Delta\sigma = \sigma_{11} - \frac{\sigma_{22} + \sigma_{33}}{2}$$

$$\text{if} |\sigma_{11} - \sigma_{iso}| \leq |\sigma_{33} - \sigma_{iso}| \Delta\sigma = \sigma_{33} - \frac{\sigma_{22} + \sigma_{11}}{2}$$

and

c) The asymmetry parameter (•), which has given by:

$$\text{If} \quad |\sigma_{11} - \sigma_{iso}| \geq |\sigma_{33} - \sigma_{iso}| \eta = \frac{\sigma_{22} - \sigma_{33}}{\delta}$$

$$\text{If} \quad |\sigma_{11} - \sigma_{iso}| \leq |\sigma_{33} - \sigma_{iso}| \eta = \frac{\sigma_{22} - \sigma_{11}}{\delta}$$

It is useful to define the span (Ω), and the skew (κ) of a CSA tensor. The span is defined as:

$$\Omega = \sigma_{33} - \sigma_{11}$$

and indicates the width of the NMR line shape for a nonspinning, stationary, sample . The skew is defined as:

$$\kappa = \frac{3(\sigma_{iso} - \sigma_{22})}{\Omega}$$

The main structures in JackfruitEthyl isovalerate, Propyl isovalerate ,Isobutyl isovalerate and 3-methyl butyl acetate with effective sides including different atoms[62-64].

Using the theoretical software, it is possible to show the chemical structure of the molecules that have main role in the anti-cancer effect of Jackfruit. NMR parameters have calculated by Gaussian 03 program at DFT level of theory[65].

RESULTS AND DISCUSSION

Nuclear magnetic resonance study depicts the physical insight into the influenceof differentstructures.In this work NMR parameters were calculated the Ethyl isovalerate ,Propyl isovalerate ,Isobutyl isovalerate and 3-methyl butyl acetate extracted of Jackfruit with different functional groups in their active sites that the consider models geometry optimization were accomplished by method DFT by standard basis set (6-31 G*) are employed to calculate the CS tensor. The CS tensors have calculated the sites of various atoms[66-69].

One of the powerful computational methods is Density functional theory (DFT), which it has applied to investigate on these epileptic drugs. In fact ,we calculate NMR factors and then compare data and We draw diagrams associated with them According to Fig.1[70-72].

Therefore, we resulted that Ethyl group substitution causes the stability of course, highlighting the vital role of Jackfruit and the Phenyl group substitution can scramble to reduce the role of atoms influences Jackfruit [73,74].

NMR calculations on Jackfruit using density functional theory (DFT) reveal that methods including electron correlation show significant improvements in the NMR shielding over results. The NMR measurements were carried out using B3LYP/6-31G* in GIAO method of nuclear magnetic resonance at theoretical concepts in different dielectric constants (Table1)[75,76].

NMR calculations on Jackfruit using density functional theory (DFT) reveal that methods including electron correlation show significant improvements in the NMR shielding over results (Table 1)[7-79].

The results of table1 are shown in fig.1 , where we plot the chemical shift (δ) and chemical shift isotropy (σ_{iso}) , asymmetry parameter (η) and shielding tensor anisotropy (Ω) and anisotropy ($\Delta\sigma$)of the Ethyl isovalerate ,Propyl isovalerate, Isobutyl isovalerate and 3-methyl butyl acetateextracted of Jackfruit with different functional

Table 1: NMR parameters (ppm) of ethyl-n-propyl disulphide ,ethanetiol, diethyl trisulphide, diethyl disulphide, propyl-2-methyl-butanoate,ethyl-2-methyl butanoate, ethyl propanoate using DFT level of theory

Ethyl isovalerate ATOM	σ_{11} σ_{22} σ_{33}	σ_{iso}	σ_{aniso}	$\Delta\sigma$	δ	η	Ω	κ
	167.0455	180.2984	20.6995	20.6995	-13.2529	-0.95	27.0526	0.06
1 C	179.7517							
	194.0981							
	114.0802	134.8035	57.1046	57.1046	-20.7233	-0.16	58.7931	0.88
2 C	117.4571							
	172.8733							
	-74.2765	114.3269	177.822	-282.9051	118.548	-0.4	-307.1514	0.68
3 O	184.3823							
	232.8749							
4 C	-70.6721	24.2061	99.7716	-142.3173	66.5144	-0.57	-161.3926	0.52
	52.57							
	90.7205							
	129.754	148.592	32.7999	32.7999	-18.838	-0.83	40.7046	0.22
5 C	145.5633							
	170.4586							
6 C	156.7358	163.4304	11.9981	11.9981	-6.6946	-0.8	14.6934	0.26
	162.1264							
	171.4292							
7 C	162.2208	173.1488	29.6363	29.6363	-10.928	-0.19	30.6855	0.86
	164.3192							
	192.9063							
8 O	-420.0033	-118.442	634.2107	634.2107	-301.5613	-0.59	724.3685	0.5
	-239.6878							
	304.3652							
9 C	152.8327	169.8692	37.0852	37.0852	-17.0365	-0.54	41.76	0.55
	162.1822							
	194.5927							
10 H	27.6587	31.7445	9.8921	9.8921	-4.0858	-0.38	10.6806	0.7
	29.2356							
	38.3393							
11 H	27.3295	31.2692	7.6624	7.6624	-3.9397	0.38	9.048	-0.7
	30.1007							
	36.3775							
12 H	27.5315	31.2791	8.2253	8.2253	-3.7476	0.56	9.2311	-0.53
	29.5431							
	36.7626							
13 H	23.5975	28.6156	6.9449	-7.52715	4.63	-0.91	-9.6481	0.12
	29.0039							
	33.2456							
14 H	23.7434	28.6882	6.3775	-7.1472	4.2517	-0.83	-9.1965	0.22
	29.3813							
	32.9399							

15 H	27.8549	30.9577	4.7711	4.7711	-3.1028	-0.97	6.2835	0.03
	30.8798							
	34.1384							
16 H	26.2791	30.2155	-5.904	3.2059	4.8089	-0.77	-7.1423	0.30
	30.9459							
	33.4214							
17 H	26.8755	30.5414	6.8917	6.8917	-3.6659	-0.74	8.2604	0.33
	29.6129							
	35.1359							
18 H	27.7324	31.746	9.6515	9.6515	-4.0136	-0.39	10.4479	0.69
	29.3252							
	38.1803							
19 H	26.4291	31.5072	-7.6171	4.9185	7.3778	-0.96	-9.9966	0.04
	31.6667							
	36.4257							
20 H	29.1892	31.881	7.8726	7.8726	-2.6918	-0.05	7.9402	0.96
	29.3244							
	37.1294							
21 H	27.4803	31.5561	9.6027	9.6027	-4.0758	-0.42	10.4776	0.66
	29.23							
	37.9579							
22 H	27.3606	31.6318	9.18545	9.18545	-4.2712	-0.56	10.3948	0.53
	29.7793							
	37.7554							
23 H	28.6499	31.8327	7.6604	7.6604	-3.1828	-0.39	8.2897	0.69
	29.9086							
	36.9396							
Propyl	isovalerate							
	158.9734	172.8271	32.6236	32.6236	-13.8537	-0.43	35.6028	0.66
1 C	164.9318							
	194.5762							
	160.4815	167.7261	8.2955	10.86695	5.5304	-0.69	-12.775	0.134
2 C	169.4404							
	173.2565							
	130.1276							
3 C	140.3444	150.9497	47.1411	47.1411	-20.8221	-0.4	52.2495	0.6
	182.3771							
4 C	-69.084	24.4338	93.8795	-140.27	62.5864	-0.5	-156.1042	0.59
	55.3654							
	87.0202							
	-73.4017	114.5995	183.7294	-282.0018	122.4863	-0.4	-310.4875	0.6
5 O	180.1144							
	237.0858							
6 C	105.4598	129.0033	58.9091	-23.5435	58.9091	-0.3	62.8162	0.7
	113.274							
	168.276							
7 C	156.615	171.4555	17.9275	-22.2607	11.9516	-26.7921	0.3	-0.7
	174.3443							
	183.4071							
8 C	176.0885	183.4517	18.9782	18.9782	-7.3632	-0.2	20.0153	0.3

	178.1627							
	196.1038							
9 C	152.9712	170.9333	35.88	35.88	-17.9621	-0.6	41.7413	0.4
	165.1162							
	194.7125							
10 O	-403.3782	-102.6027	649.7776	649.7776	-300.7755	-0.5	733.9606	0.5
	-235.0122							
	330.5824							
11 H	26.0381	31.2547	7.4231	-7.8253	4.9496	-0.9	-10.1662	0.07
	31.5225							
	36.2043							
12 H	27.6513	31.7338	9.8435	9.8435	-4.0825	-0.3	10.6448	0.6
	29.2539							
	38.2961							
13 H	29.326	32.2089	7.5015	7.5015	-2.8829	-0.2	7.8839	0.8
	30.0909							
	37.2099							
14 H	26.6209	30.3656	6.9879	6.9879	-3.7447	-0.7	8.4033	0.3
	29.4518							
	35.0242							
15 H	26.6004	30.5521	-1.3378	3.3136	4.9705	-0.8	-7.2653	0.2
	31.1901							
	33.8657							
16 H	25.3225	30.2895	7.45055	3.7997	5.6994	-0.6	-6.1344	0.5
	31.4569							
	34.0892							
17 H	23.5498	28.6475	-7.6466	3.6354	5.453	-0.5	-8.7331	0.5
	30.11							
	32.2829							
18 H	23.7662	28.7316	7.44815	3.7707	5.656	-0.6	-8.7361	0.4
	29.9264							
	32.5023							
19 H	26.1107	30.9366	-7.2389	4.8219	7.2328	-0.9	-9.6478	0.001
	30.9407							
	35.7585							
20 H	26.1443	30.9350	7.1149	-7.1861	4.7433	-0.9	-9.534	0.014
	30.9825							
	35.6783							
21 H	27.2576	31.6356	10.2752	10.2752	-4.378	-0.4	11.2281	0.6
	29.1635							
	38.48857							
22 H	27.6459	31.8436	8.7526	8.7526	-4.1977	-0.6	10.0328	0.4
	30.2063							
	37.6787							
23 H	27.6818	31.8435	8.8312	8.8312	-4.1617	-0.5	10.0492	0.5
	30.1179							
	37.731							
24 H	27.5354	31.7909	9.5295	9.5295	-4.2555	-0.5	10.6085	0.5
	29.6934							
	38.1439							

25 H	27.4469	31.6369	9.6935	9.6935	-4.19	-0.4	10.6524	0.6
	29.3646							
	38.0993							
26 H	28.6559	31.8611	7.5576	7.5576	-3.2052	-0.4	8.2436	0.6
	30.0279							
	36.8995							
Isobutyl isovalerate								
	159.6475	174.6741	32.7109	32.7109	-15.0266	-0.5	36.8338	0.55
1 C	167.8934							
	196.4813							
	156.2917	164.958	11.2647	-12.9994	7.5098	-0.8	-16.1761	0.6
2 C	166.1145							
	172.4678							
	103.3796	124.3478	48.668	48.668	-20.9682	-0.4	53.4135	0.6
3 C	112.8707							
	156.7931							
4 O	-70.7403	115.3705	176.7299	-279.16625	117.82	-0.4	-303.9308	0.59
	183.6614							
	233.1905							
	-68.7146	24.3574	93.3855	-139.608	62.257	-0.5	-155.329	0.6
5 C	55.1724							
	86.6144							
6 C	130.019	150.9023	47.4955	47.4955	-20.8833	-0.4	52.5469	0.3
	140.1218							
	182.5659							
7 C	160.7862	167.8329	8.2883	-10.57015	5.5256	-0.7	-12.5723	0.6
	169.3542							
	173.3585							
8 C	158.9422	172.8881	32.4353	32.4353	-13.9459	-0.4	35.5694	0.6
	165.2104							
	194.5116							
9 C	161.0028	174.0359	29.6648	29.6648	-13.0331	-0.4	32.8097	0.6
	167.2926							
	193.8125							
10 O	-403.9463	-102.8885	649.007	649.007	-301.0578	-0.5	733.7291	0.53
	-234.5021							
	329.7828							
11 C	152.9529	170.9497	35.7014	35.7014	-17.9968	-0.6	41.7977	0.4
	165.1454							
	194.7506							
12 H	27.3774	31.6348	9.6151	9.6151	-4.2584	-0.4	10.6685	0.6
	29.4831							
	38.0449							
13 H	28.534	31.9367	7.8822	7.8822	-3.4027	-0.4	8.6575	0.6
	30.0846							
	37.1915							
14 H	27.2533	31.73	9.8673	9.8673	-4.4767	-0.5	11.0549	0.57
	29.6285							
	38.3082							
15 H	27.4221	30.6495	7.0295	7.0295	-3.2274	-0.5	7.9138	0.55

	29.1206							
	35.3359							
16 H	24..3723	28.8883	-6.774	3.1498	4.7247	-0.5	-7.6658	0.53
	30.2545							
	32.0381							
17 H	23.257	28.7341	-8.2157	3.5559	5.3338	-0.4	-9.033	0.6
	30.6554							
	32.29							
18 H	26.4044	30.5168	-6.16855	3.596	0.2	5.394	-0.8	-7.7084
	31.0331							
	34.1128							
19 H	25.2507	30.2666	-7.52385	3.6699	5.5048	-0.6	-8.6858	0.4
	31.6126							
	33.9365							
20 H	26.5389	30.3707	7.0441	7.0441	-3.8318	0.7	8.5279	0.3
	29.5065							
	35.0668							
21 H	27.5788	31.7291	9.9302	9.9302	-4.1503	-0.4	10.7705	0.6
	29.2593							
	38.3493							
22 H	26.0681	31.2378	-7.7546	-5.1697	7.3096	-0.8	-10.0428	0.08
	31.5345							
	36.1109							
23 H	29.2799	32.1936	7.3881	7.3881	-2.9137	-0.3	7.8391	0.7
	30.1818							
	37.119							
24 H	25.4211	30.9802	8.2637	-8.3012	-0.9	-11.0433	5.5092	0.006
	36.4644							
	30.9552							
25 H	27.6723	31.7613	9.5543	9.5543	-4.089	-0.4	10.45585	0.6
	29.4809							
	38.1308							
26 H	29.4561	32.084	7.5547	7.5547	-2.6279	-0.08	7.6644	0.9
	29.6755							
	37.1205							
27 H	27.3943	31.6344	9.7831	9.7831	-4.2401	-0.4	10.7622	0.6
	29.3524							
	38.1565							
28 H	27.4984	31.7839	9.5726	9.5726	-4.2855	0.5	10.6672	0.55
	29.6876							
	38.1656							
29 H	28.5979	31.855	7.5287	7.5287	-3.2571	-0.4	8.2762	0.6
	30.0929							
	36.8741							
3-methyl butyl acetate								
	160.3517	172.8579	30.8971	30.8971	-12.5062	0.3	33.1043	0.73
1 C	164.7661							
	193.456							
	161.9293	166.2575	8.4653	8.4653	-4.3282	-0.69	9.9718	0.39
2 C	164.9422							

	171.9011							
	136.8526	157.111	37.2188	37.2188	-20.2584	-0.77	45.0709	0.3
3 C	152.5568							
	181.9235							
4 C	106.823	130.4165	58.1738	58.1738	-23.5935	-0.35	62.376	0.69
	115.2274							
	169.199							
	-71.1458							
5 O	189.3192	118.3985	177.3985	-284.3165	118.6237	-0.4	237.0222	0.69
	237.0222							
6 C	-67.1794	27.5751	-142.1318	61.7492	92.6237	-0.4	-156.5037	-0.63
	60.5805							
	89.3243							
7 C	157.7092	172.9963	43.4201	43.4201	-20.2871	-0.57	49.2339	0.52
	164.3367							
	201.9431							
8 C	149.6863	169.166	38.2829	38.2829	-19.4797	-0.68	45.0013	0.4
	163.1237							
	194.6879							
9 O	-424.0903	-121.1512	631.279	631.279	-302.9391	-0.6	723.7918	0.48
	-239.0648							
	299.7015							
10 H	26.0171	31.4654	8.471	8.471	-5.4483	-0.26	11.0957	0.053
	31.2664							
	37.1128							
11 H	29.2571	31.9948	7.5085	7.5085	-2.7377	-0.17	7.7433	0.87
	29.7267							
	37.0004							
12 H	27.4985	31.6956	9.5651	9.5651	-4.1971	-0.48	10.5738	0.61
	29.5159							
	38.0723							
13 H	27.847	31.0362	6.9495	6.9495	-3.1892	-0.54	7.8222	0.55
	29.5923							
	35.6692							
14 H	27.4546	31.1441	-5.5342	3.0421	4.5632	-0.78	-6.7316	0.28
	31.7914							
	34.1862							
15 H	25.791	30.882	-7.6364	4.0901	34.1862	-0.75	-9.1811	0.32
	31.8827							
	34.9721							
16 H	23.7861	28.8168	-7.54615	3.0779	4.6168	-0.36	-8.1086	0.72
	30.7698							
	31.8947							
17 H	22.4908	28.4087	-8.8768	4.643	6.9645	-0.72	-10.5609	0.36
	29.6836							
	33.0517							
18 H	26.7819	30.5241	6.35805	6.35805	-3.7422	-0.86	7.9809	0.18
	30.0276							
	34.7628							

19 H	26.8316	30.5145	6.5099	6.5099	-3.6829	-0.82	8.0229	0.24
	29.8575							
	34.8545							
20 H	27.3998	31.1733	8.2724	8.2724	-3.7735	-0.53	9.2885	0.56
	29.4319							
	36.6883							
21 H	27.3815	31.6280	9.2758	9.2758	-4.2465	-0.54	10.4304	0.55
	29.6907							
	37.8119							
22 H	27.425	31.6041	9.6168	9.6168	-4.1791	-0.46	10.5903	0.63
	29.372							
	38.0153							
23 H	28.7529	31.7589	7.36055	7.36055	-3.006	-0.36	7.913	0.72
	29.8578							
	36.6659							

groups in their active sites[80,81].

We have found that the O and S atoms denoted has maximal shift in all compounds and other indicated atoms almost have the similar shifts in different structures (Fig.1). This shows the significant role of these atoms, in the above mentioned molecules, on anti-cancer characteristics of Jackfruit[82-84].

Also, the graphs of HNMR and CNMR based on isotropic magnetic shielding constants σ_{iso} (ppm), anisotropic magnetic shielding tensors σ_{aniso} (ppm) and Chemical shifts ´ (ppm) for effective compoun -CNT systems are listed in Figs2,3 [85-88].

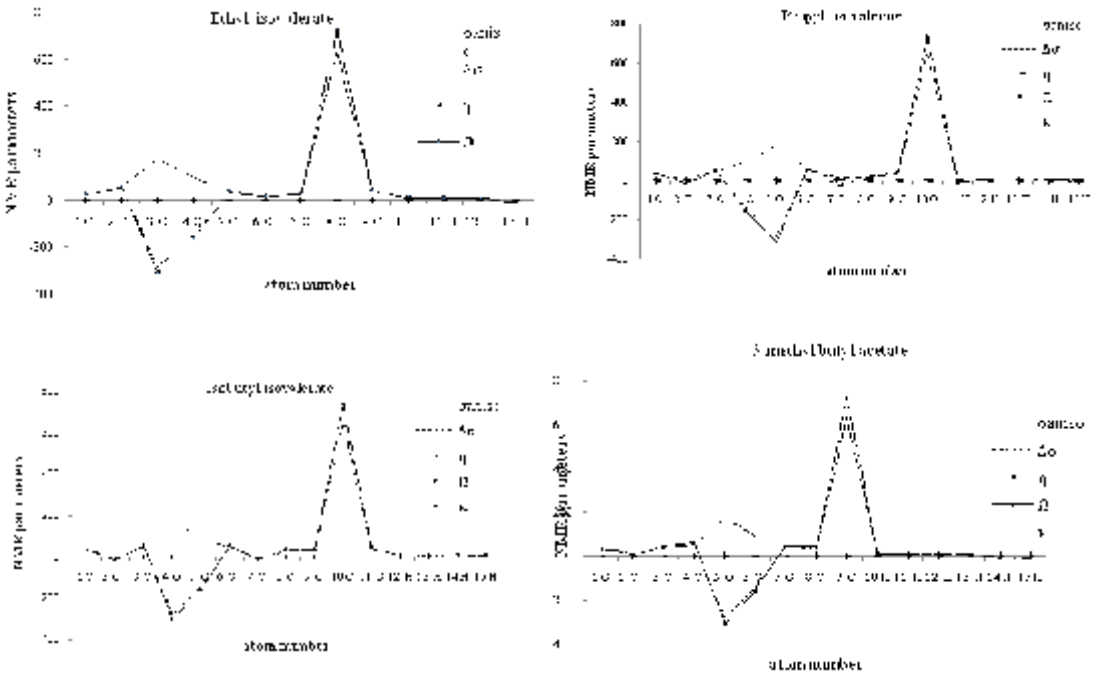
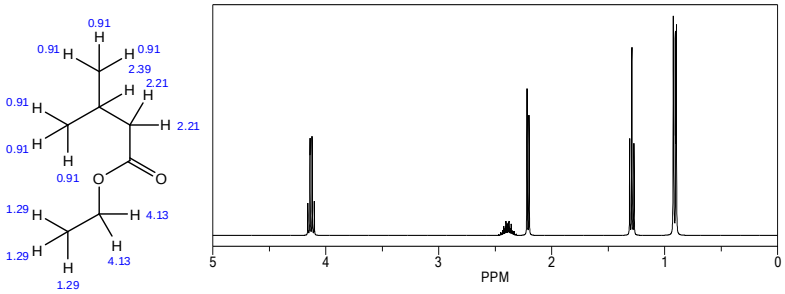
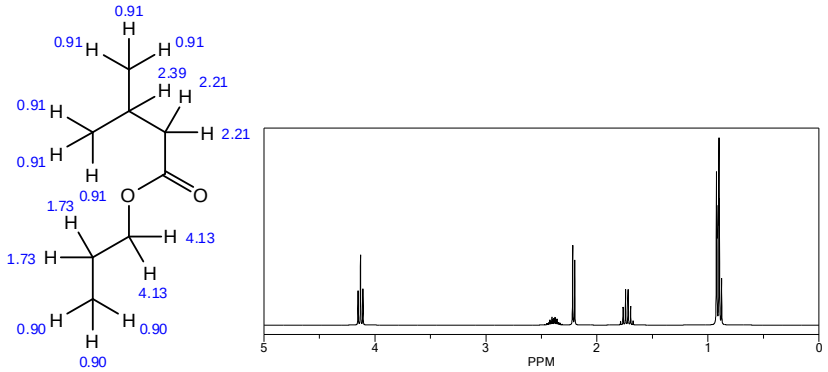


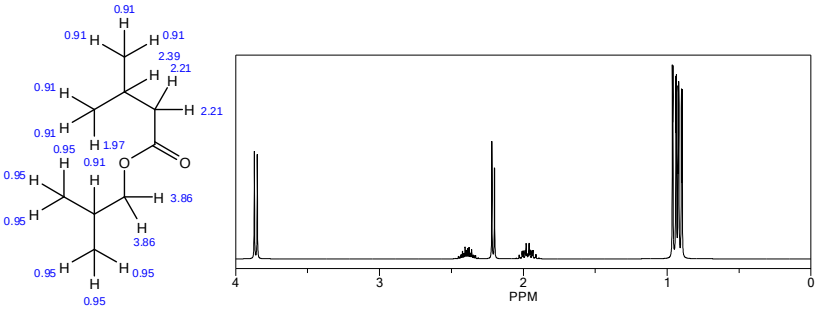
Fig. 1: NMR parameters of Ethylisovalerate ,Propyl isovalerate ,Isobutyl isovalerate and 3-methyl butyl acetateversus different atoms in active sites using DFT level of theory



Propyl isovalerate



Isobutyl isovalerate



3-methyl butyl acetate

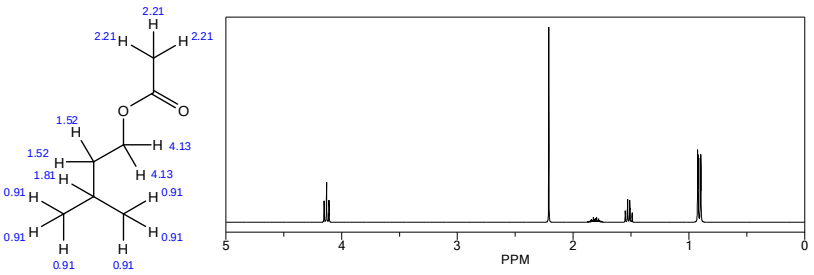
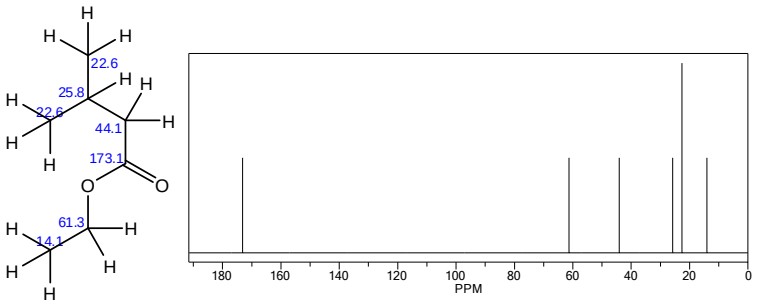
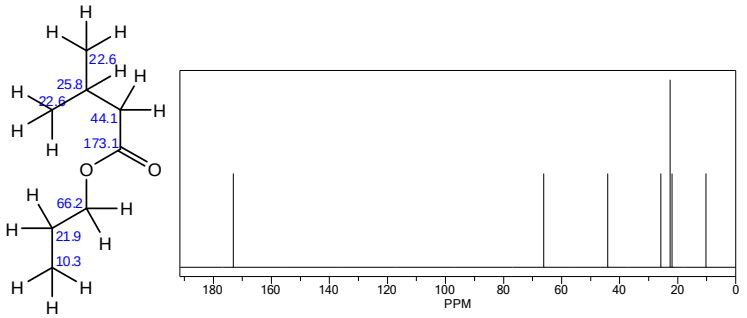


Fig. 2: Results of NMR ^{1}H for Ethylisovalerate ,Propyl isovalerate, Isobutyl isovalerate and 3-methyl butyl acetate

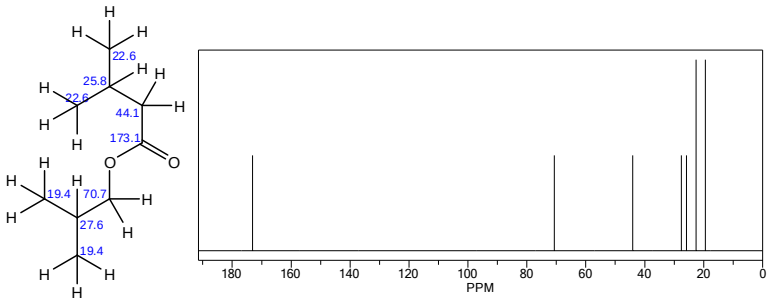
Ethyl isovalerate



Propyl isovalerate



Isobutyl isovalerate



3-methyl butyl acetate

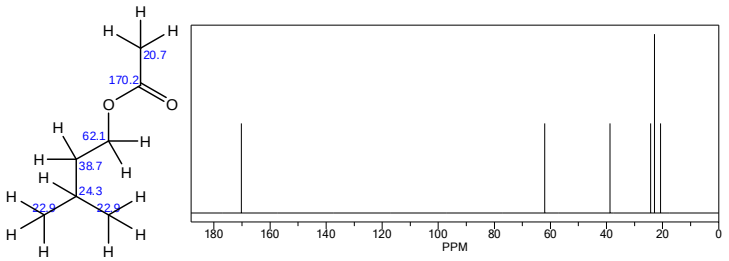
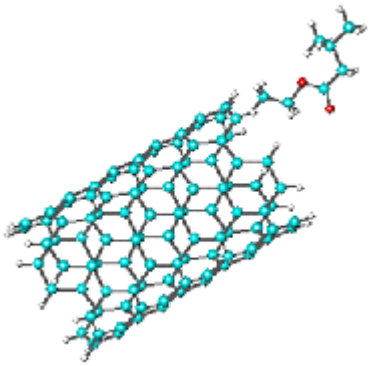
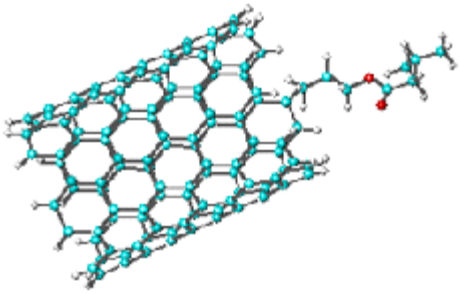


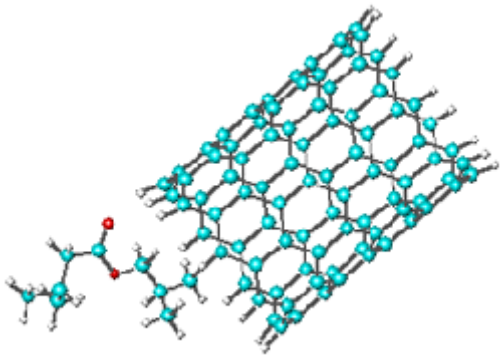
Fig. 3: Results of NMR ^{13}C for Ethylisovalerate ,Propyl isovalerate,Isobutyl isovalerate and 3-methyl butyl acetate



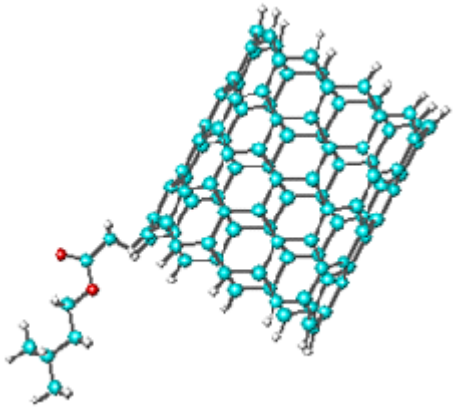
CNT (5,5)Armchair-Ethyl isovalerate



CNT (6,6)Armchair- Propyl isovalerate



CNT (9,0)Zigzag-Isobutyl isovalerate



CNT (10,0)Zigzag-3-methyl butyl acetate

Fig.4: Optimized structures of different carbon nanotubes bonded to Ethylisovalerate ,Propyl isovalerate ,Isobutyl isovalerate and 3-methyl butyl acetate

The results of the above observations strongly suggest that the different data observed in the effective compounds- SWCNT is predominantly due basis set functions, induced by a change in active sides of the various structures (Fig.4)[89-93].

CONCLUSION

Use of the different structures for characterization of motions and determination of the properties or dynamics of the molecules of interest requires a number of theoretical or computational steps and all of which are current activities of research, Therefore in this paper we summarize the method and describing the reasons for the choices.

To conclude, we have performed simulations and solvent NMR of theoretical methodology on Ethyl isovalerate ,Propyl isovalerate ,Isobutyl isovalerate and 3-methyl butyl acetateextracted of Jackfruit with different functional groups in their active sites. Our calculations have demonstrated that such extrapolation schemes significantly overestimate the effective compounds-SWCNT shifts that the O and S atoms were the most active point at indicated structure.

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