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The Theoretical Study on a Nano Biosystem Consisting of Nano Tube-Catalytic Site of Bacillus Subtilis α-Amylase, PDB: 1UA7

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Abstract:
α-Amylase has been studied extensively from various sides. This enzyme is used in many industries .Many applications of this enzyme have encouraged us for greater attempts on the study of α-amylase and to search for more effective processes. In this investigation, the structure of nanotube - catalytic site of bacillus subtilis α- amylase was optimized by hyperchem 7.0 and then it was investigated with ab initio/hartree fock and density functional theory /B3LYP methods using the STO-3G, 3-21G and 6-31G basis sets for a physicochemical explanation of interactions within these nano biosystem. Then nuclear Magnetic Resonance (NMR) parameters and so charge, dipole moment, and stability energy were calculated on the optimized structure. We have found each of active atoms that indeed play an important role in imparting extra stability. In the current study, we have reported the NMR parameters of 8 atoms of catalytic site of bacillus subtilis alpha-amylasethe. Interesting finding of the present study is that in NMR shielding for each of active atoms, O_8 and O_{14} had maximal shift in all of levels. In catalytic mechanism of this enzyme, O_{14} is adopting a chair structure leading to the easy cleavage of the glucoside bond (fixer for catalysis). This investigation suggests that nanotube interactions in this nano biosystems indeed play an important role in imparting extra stability of the catalytic site of the enzyme .Energy parameters in B3LYP level in different basis sets have more negative values than HF and have indicated the most stability in B3LYP6-31/G level and so dipole moment in this structure have observed that in HF3-21/G is maximum. The aim of this work was to discuss the aspects of the electronic structure of this nano biosystem to increase their advantages in practical applications.
Keywords: *Nanotube-catalytic site, Bacillus subtilis α-amylase, AB initio, DFT, NMR shielding, GIAO, CSGT, HF, B3LYP.*

1. INTRODUCTION

α -Amylase (α-1, 4-glucan-4-glucanohydrolase, EC 3.2.1.1) catalyzes the hydrolysis of D-(1, 4)-glycosidic linkages in polysaccharides such as starch, glycogen, and malto oligosaccharides, so that produces anomeric products [1]. This enzyme has been studied extensively from various sides, including structure, function, secretion, and industrial application. α-Amylases are the most widely studied members of the glycosyl hydrolase family 13 [1,2].

Microorganisms such as bacteria and fungi have been extensively screened for suitable α-amylase production. Several extracellular α -amylases are of prominent industrial importance [3].

This enzyme is extensively used in many industries including brewing, starch liquefaction, food, textile, paper and pharmaceuticals. These uses encourage us for greater attempts on increasing to

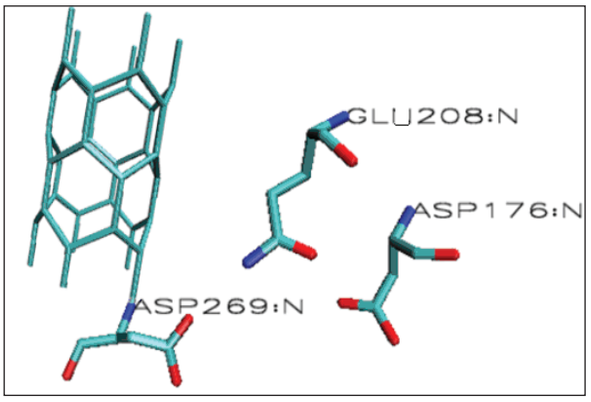


Figure 1: *The structure of nanotube –catalytic site of bacillus subtilis α amylase in VMD software.*

study α-amylases and to search for more effective processes [4-5].

Today NMR spectroscopy is a powerful tool in chemistry and bio chemistry [6-7]. In quantum mechanics, the quantity is directly related with the NMR chemical shift. The shielding is defined as the mixed second derivative of the energy with respect to magnetic moment of the nucleus and the strength of the applied magnetic field. It is solved through the second-order perturbation theory with the Zeeman Hamiltonian, treated as a perturbing term [8-9].

The methods currently employed for calculating of the NMR shielding are done by ab initio method consist of the Hartree Fock (HF) [10] and so density functional theory (B3LYP) levels. [11-13]. The term "AB initio" refers to calculations that are considered directly from theoretical principles, without inclusion of experimental data [14].

Gaussian basis sets are normally employed as the basis functions to fit the electronic orbital in a molecule [15]. The NMR shielding at very accurate levels of approximation are available in literature .The widely used methods for calculating of chemical shifts are as follows: GIAO and CSGT approximations [16-19]. The GIAO approach is known to give satisfactory shielding for different nuclei with larger molecules [17-19].

This study have surveyed the active atoms which play in stability by examining the NMR shielding. Also optimum energy and dipole moment were evaluated. The aim of this work is to discuss the aspects of the electronic structure of this nano biosystem and to increase their advantages in practical applications.

1.2. Computational methods

The zigzag single-walled carbon nanotubes (SWCNT) with (5, 0) structure were made using the implement in HyperChem7.0. The nanotube symmetry is D_{5d} [20, 21].

In this study, a structure of nanotube –catalytic site of bacillus subtilis α amylase was made by HyperChem7.0 (Figures 1, 2). The structure of this enzyme is deposited in Protein Data Bank as 1UA7. At first, nanotube –catalytic site of enzyme was optimized. The Gaussian 98 was used for all calculations [22] and then Nuclear Magnetic Resonance (NMR) parameters by AB initio (hartree fock) and density Functional Theory (B3LYP) methods was calculated on the optimized structure (Figure 2.) by GIAO and CSGT methods using the STO-3G ,3-21G and 6-31G basis sets .The results of the hartree fock and B3LYP methods of NMR shielding values (ppm) including isotropic (σ_{iso}) and anisotropic (σ_{aniso}) effects and so charge , energy (kcal/mol) and dipole moment (debye) parameters for 8 number of active atoms of catalytic site were reported.

2. RESULTS AND DISCUSSION

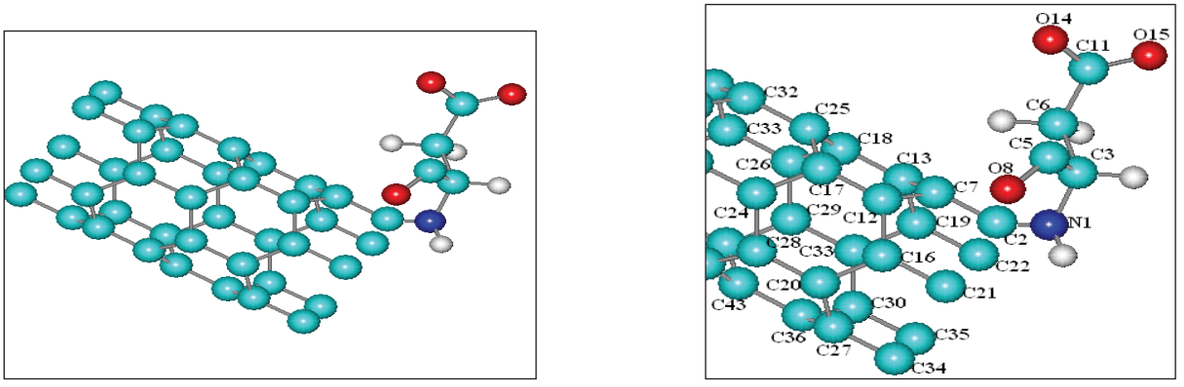
In the current study, we performed the structural computations on the nanostructure of the nanotube-catalytic site system of bacillus subtilis α amylase.

In this investigation, we analyze and report the NMR shielding values of 8 atoms of catalytic site at HF and B3LYP levels by STO-3G, 3-21G and 6-31G basis sets. We have studied principle calculations on this nanostructure.

The NMR parameters are given in Table 1 and 2. Also, parameters of σiso and σaniso of mentioned atoms versus atom number and charge is shown in Figure 3, 4.

The results of Table 1 are shown in Figure 3 and 4, where we plot the NMR shielding isotropy (σ_{iso}) and NMR shielding anisotropy (σ_{aniso}) of the nanotube-catalytic site for each of active atoms.

We found that O_8 and O_{14} had maximal shift. Other



(a) ***(b)***

Figure 2: *The geometrical structure of the optimized structure atoms*

indicated atoms had the similar shifts in different positions therefore some atoms on nanotube-catalytic site of bacillus subtilis alpha amylase indeed play an important role in imparting extra stability and functionality and the best interaction in the catalytic site of the enzyme.

It should be noted that Calculations at the B3LYP and HF levels in CSGT and GIAO methods have shown that shielding properties in6-31 G is better than the other basis sets, (Figures 3a, 3b, 3c, 3d).

In catalytic mechanism of this enzyme, one hydrogen-bonding is between O_{14} of carboxyl group of ASP269 and sugar in the catalytic subsite -1 in the enzyme/ acarbose. This atom is adopting a chair structure leading to the easy cleavage of the glucoside bond) fixer for catalysis. [23,1] The interesting finding of the present study is that O_8 and O_{14} have maximal shift in B3LYP levels.

In the course of parameters deliberation and relating them to the fundamental electronic structure of the considered system, σaniso and σ_{iso} parameters effects provided beneficial information on the interaction characteristics.

The graphs of the charge value versus the isotropic and anisotropic parameters at B3LYP /6-31G and HF /6-31G Levels in Figure 4 shows charge Density is high on O_8 and O_{14}.

Also, we have detected the electromagnetic nature of this system by calculating the parameters consisting energy and dipole moment which provide valuable information on the interaction characteristics.

By plotting the energy values versus basis sets, it is observed that stability energies decrease linearly in basis sets consisting STO – 3 G, 3 - 21 G and 6 - 31 G in HF and B3LYP levels, respectively (Figure 5). Also, B3LYP/6-31G (5b) is better than the other level/basis sets (Table 2).

The factors such as dipole moment values are very important quantities for determining and estimating polarity of component [24]. The dipole moment values of this system are reported in Table 2 and Figure 5a.

In this nano biosystem, it was observed that dipole moment value in HF/3-21G was maximum. Therefore maximum polarity was observed in this level.

Enzymes are big structures that cannot directly be utilized by QM methods (quantum mechanics methods). Only the substrate and residues in the catalytic site are treated quantum mechanically and the rest of the enzyme is explained at the MM method (molecular mechanics methods). This decreased the computational dispersion and made it possible to investigate large enzyme structures [25]. The QM method is increasingly applied and is preferred to traditional methods due to their versatility and ability to describe the same system at different levels of detail. [14, 26, 27].The NMR shielding quantity has been applied to a broad range of researches in chemistry and biochemistry and has revealed to be in valuable investigations. It has played a significant role in the structural studying of protein [28-30]. AB initio calculation of NMR shielding has become an indispensable tool in the analysis of molecular structure and accurate assignment of NMR spectra of systems [7].

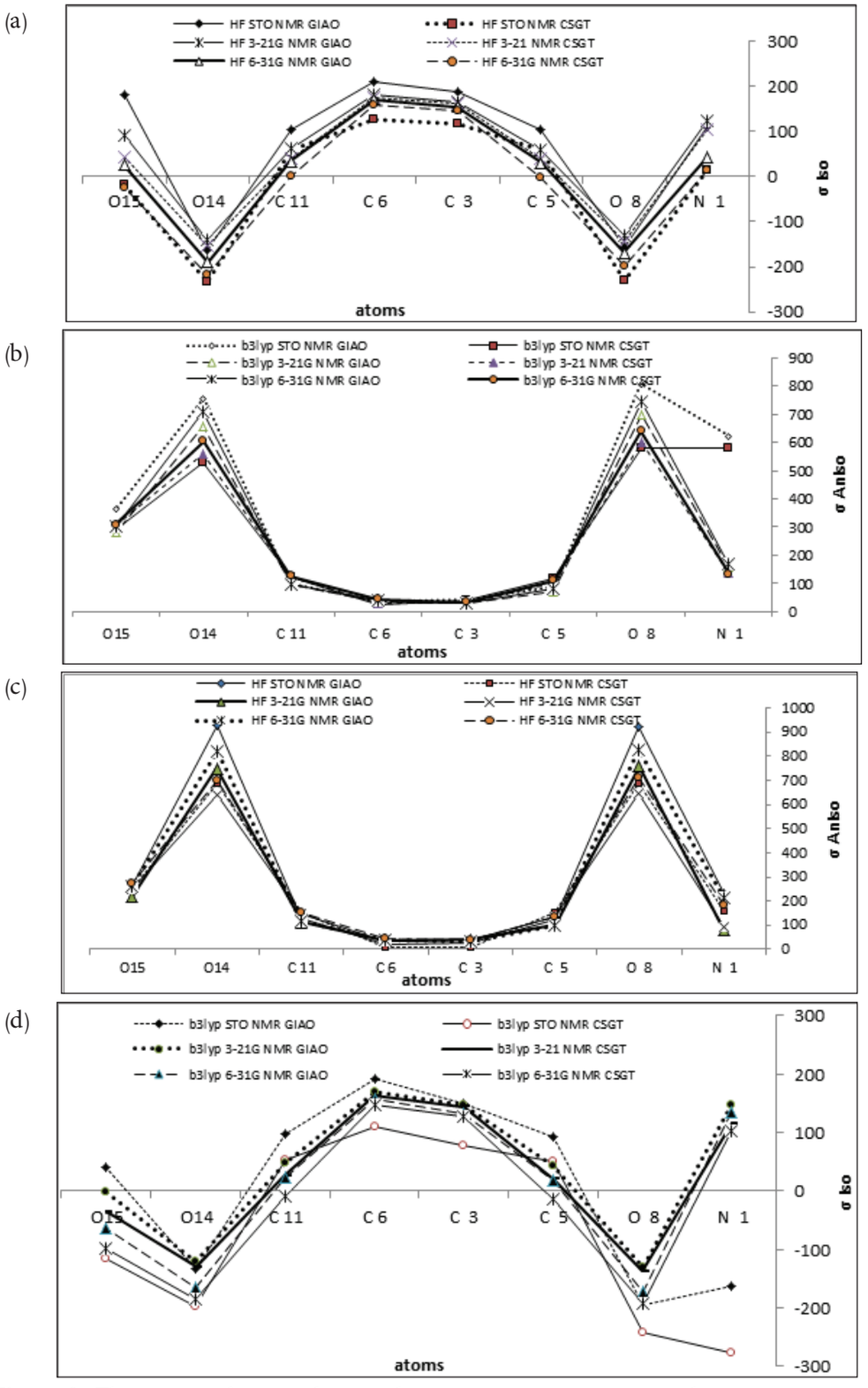


Figure 3: *The curves of nanotube- catalytic site atoms via atom number versus σiso and σaniso at HF and B3LYP levels.*

Table 1: *Parameters of active atoms of nanotube- catalytic site at the B3LYP/STO-3G,3-21G,6-31G and HF/ STO-3G,3-21G,6-31G Levels.*

ATOMS	B3LYP											
	GIAO						CSGT					
	STO		3 – 21G		6 -31G		STO		3 – 21G		6 -31G	
	σ_{iso}	σ_{aniso}	σ_{iso}	σ_{aniso}	σ_{iso}	σ_{aniso}	σ_{iso}	σ_{aniso}	σ_{iso}	σ_{aniso}	σ_{iso}	σ_{aniso}
N 1	-163.235	621.3616	146.4348	157.3295	135.2606	168.0287	-276.221	581.1101	115.881	136.5067	101.5689	134.9382
C 2	135.9311	32.9411	131.1982	82.9427	120.6172	97.6467	74.7511	34.7353	129.4735	60.402	114.5389	79.1743
C 3	148.553	42.5338	146.0495	32.4942	133.0267	31.5459	78.3224	41.302	143.5597	29.0272	126.4841	34.6713
C 5	93.081	89.2127	42.0018	71.5522	17.582	79.38	49.6104	117.9813	20.2642	100.5623	-14.4474	111.0025
C 6	192.1209	40.0372	168.3998	33.2372	157.1759	39.6962	111.2839	24.434	163.0103	30.7457	147.5556	45.0975
C 7	78.0795	202.0735	135.1696	54.3825	122.6085	59.3771	12.4847	178.4198	132.2914	36.5367	116.7211	46.4686
O 8	-193.748	807.7763	-129.709	697.2827	-172.4596	742.5682	-241.966	581.4649	-136.761	599.5016	-192.241	640.7042
C 11	97.7682	99.2683	47.7833	94.502	23.1143	95.9594	53.7782	120.8568	25.7788	120.1388	-9.4165	125.7137
C 12	97.138	136.6853	82.3399	125.3208	62.7077	137.2286	44.4758	119.1668	77.6976	123.1585	50.6841	133.9655
C 13	93.1827	128.2265	76.473	117.8205	56.2517	130.4364	44.7323	108.0565	71.9638	116.8082	44.3501	129.7741
O 14	-133.036	755.805	-121.602	658.9558	-165.8287	709.6897	-198.061	526.2749	-129.609	561.3619	-186.073	605.5115
O 15	39.6043	362.4785	-0.7055	280.6241	-63.2308	300.7571	-115.132	291.6697	-35.7916	306.7081	-99.1901	308.2451
C 20	96.039	135.1625	69.0566	150.0127	50.1006	161.3793	45.7453	112.3665	67.0356	143.2968	38.9813	154.9608
C 21	82.8682	188.7389	27.5063	174.4261	8.4275	186.2284	12.6125	207.3865	29.5641	164.3445	-0.1521	179.0666
C 22	53.7037	127.7346	39.0576	146.6515	15.9698	164.1442	6.8544	119.4389	39.4554	137.4657	6.3822	157.4598
C 23	100.9103	139.9235	77.0743	141.499	60.4253	152.9006	49.3834	112.818	72.9732	136.6441	47.8141	147.4793
C 30	104.2707	109.4422	75.6397	129.1698	59.0242	139.863	48.3087	98.9863	71.9442	122.3278	45.6962	135.1647
C 34	90.6082	140.8022	11.1733	201.3553	-15.4043	224.9962	37.1913	120.0158	17.7152	185.6686	-19.172	210.8079
C 35	77.6693	143.5763	10.6631	212.6796	-12.7201	231.8841	34.6815	116.0081	17.3626	196.8647	-17.2246	219.042
C 36	85.8589	160.2293	99.0717	105.4865	85.221	109.6783	37.9053	130.2986	94.0523	104.3446	70.6659	109.2169
C 37	91.8316	145.3379	83.8734	132.4247	65.0199	143.9492	46.2126	117.1114	79.313	132.4041	53.6092	143.7151
	HARTREE FOCK											
N 1	110.8314	233.34	123.8268	83.0939	44.1096	215.513	13.0404	156.676	103.5966	92.3058	12.8503	181.1869
C 2	73.8429	69.008	96.53	223.483	30.0232	165.8685	31.4361	121.5727	82.9794	234.2254	3.6691	197.6753
C 3	188.6997	24.8577	164.4695	40.8067	154.0698	32.2914	116.3148	7.9129	160.772	37.978	146.7343	36.3464
C 5	105.6044	124.9071	60.1544	100.8511	30.455	97.8679	58.4501	150.7764	38.9592	136.3268	-1.957	134.5238
C 6	209.8612	21.8693	180.7049	36.0878	170.7819	36.8547	126.3774	9.694	173.5584	34.581	159.3165	43.5394
C 7	164.7277	58.9038	147.0601	42.0562	132.2958	64.1321	102.0669	49.1473	137.6983	56.136	119.2373	71.2481
O 8	-155.4045	924.5198	-130.2985	758.2691	-169.237	824.0598	-229.818	685.11	-142.431	644.4	-199.632	709.3563
C 11	105.5012	130.7188	61.32	113.3502	33.9111	116.4858	58.1994	154.5915	39.5491	145.2412	1.1741	153.985
C 12	104.1284	146.8048	70.5469	174.1066	48.239	197.7538	52.6751	125.2392	69.0744	176.6809	42.6471	200.9126
C 13	103.6658	147.7272	51.3767	220.2817	44.6987	201.7407	52.37	124.8969	54.1815	219.6214	39.1073	203.5733
O 14	-161.5206	930.7151	-140.3035	749.6197	-189.873	817.4379	-233.824	688.0354	-152.089	638.7368	-218.139	698.1294
O 15	181.5189	260.6543	91.0292	219.9559	25.302	259.183	-17.7506	246.25	41.8518	249.9586	-26.2179	270.5309
C 20	106.6339	149.667	89.3594	158.346	62.5997	196.2433	53.2035	131.2261	85.1897	167.1417	54.7362	205.3516
C 21	-389.436	374.8036	-358.9343	352.2915	-434.584	367.8849	-405.434	337.7987	-365.552	347.3916	-442.946	337.0783
C 22	-389.9936	380.5625	-490.4076	571.052	-437.946	372.8868	-405.847	343.0878	-499.009	529.1592	-446.146	358.4806
C 23	106.4162	149.8695	670.0542	1352.554	62.0515	196.7477	53.0441	131.1893	615.7786	1284.842	54.4928	205.7877
C 30	109.4672	121.6144	92.1921	149.6937	54.2053	178.9565	28.9383	164.224	88.5809	160.3818	33.3942	202.267
C 34	-395.147	385.9614	-588.3015	659.8322	-470.768	379.5589	-410.188	346.8347	-572.221	608.5003	-476.579	365.8087
C 35	-395.0097	386.2259	70.0975	222.8975	-470.226	380.1627	-410.086	347.1634	75.2154	219.2989	-476.169	366.406
C 36	107.0746	149.8616	77.9716	123.6905	62.462	200.3463	53.6575	131.0837	79.3553	118.1768	55.3587	207.9715
C 37	113.7753	124.6668	73.5419	171.8759	55.1118	156.9315	66.087	95.046	57.7555	192.3112	47.2048	147.4935

Table 2: *Parameters of active atoms consisting charge , dipole moment(DEBYE) and stability energy (kcal/mol)of nanotube- catalytic site of bacillus subtilis α-amylase at the B3LYP/STO-3G , 3-21G,6-31G and HF/ STO-3G , 3-21G , 6-31G levels.*

ATOMS	B3LYP									HF								
	STO-3G			3-21G			6-31G			STO-3G			3-21G			6-31G		
	CHARG	DIPOL MOMENT (DEBYE)	ENERGY (kcal/mol)	CHARG	DIPOL MOMENT (DEBYE)	ENERGY (kcal/mol)	CHARG	DIPOL MOMENT (DEBYE)	ENERGY (kcal/mol)	CHARG	DIPOL MOMENT (DEBYE)	ENERGY (kcal/mol)	CHARG	DIPOL MOMENT (DEBYE)	ENERGY (kcal/mol)	CHARG	DIPOL MOMENT (DEBYE)	ENERGY (kcal/mol)
N 1	-0.18003	2.1685	-1213318.5012	-0.497793	3.2424	-1221913.64601	-0.458352	4.0165	-1228320.79423	-0.239833	3.0001	-1205511.18025	-0.923615	5.3469	-1213921.25562	-0.494767	5.1235	-1220270.68134
C 2	0.05704			0.085438			0.01651			0.165417			0.823603			0.295946		
C 3	-0.024086			-0.148689			-0.054622			0.026163			-0.142692			-0.158104		
C 5	0.221558			0.685739			0.53538			0.320231			0.959748			0.824423		
C 6	-0.16257			-0.482027			-0.344409			-0.1388			-0.560369			-0.412491		
C 7	0.02226			-0.000033			-0.042704			-0.053631			-0.084162			-0.036084		
O 8	-0.164312			-0.430644			-0.356568			-0.219119			-0.519805			-0.466302		
C 11	0.224084			0.661743			0.520093			0.320594			0.889295			0.760873		
C 12	-0.012439			0.050002			0.066917			0.028383			0.101641			0.087193		
C 13	-0.001509			0.115518			0.086976			0.034283			0.120679			0.120393		
O 14	-0.174627			-0.422385			-0.344779			-0.216273			-0.521668			-0.455997		
O 15	-0.151967			-0.493079			-0.458081			-0.242246			-0.698925			-0.673054		
C 20	-0.000516			0.035489			-0.009349			0.031037			0.08873			0.085093		
C 21	-0.031827			0.045208			0.088525			0.092753			0.217787			0.174767		
C 22	0.003623			0.026849			0.069636			0.098846			0.155698			0.194083		
C 23	0.003724			0.057862			-0.007717			0.031492			0.114309			0.082379		
C 30	-0.006501			-0.043058			-0.000336			-0.138238			0.091117			-0.317247		
C 34	0.016495			0.006476			-0.025107			0.101653			0.143629			0.200388		
C 35	0.011574			0.003517			-0.017151			0.10186			0.119543			0.201033		
C 36	0.002794			0.039408			-0.004299			0.031445			0.034194			0.088635		
C 37	0.008171			0.000506			0.014797			0.002691			-0.38627			0.029044		

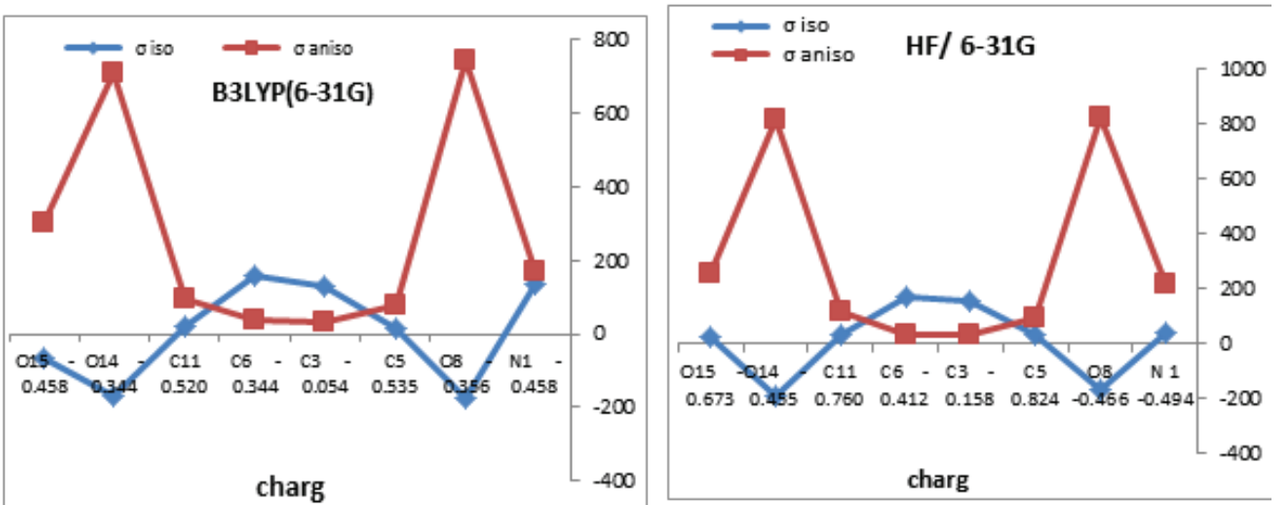


Figure 4: *Graphs of the charge value versus the isotropic and anisotropic parameters at (a) B3LYP /6-31G and (b) HF /6-31G Levels.*

The studying of nanometer sized structures will lead to products which are multi-functional.
Therefore, the studying of qualities of structures at the nano scale with the assistance of computational calculations is important to plan the specific material properties [7, 31, 32].

3. CONCLUSION

1. In the current study, we analyzed the NMR parameters of 8 atoms of catalytic site of bacillus subtitles alpha-amylase at HF and B3LYP levels with STO-3G, 3-21G and 6-31G basis sets. The results of NMR shielding for each of active atoms, showed that O_8 and O_{14} had maximal shift. This investigation suggests that some interactions on this nano biosystems indeed play an important role in imparting extra stability and functionality of enzyme.
2. In catalytic mechanism of this enzyme, O_{14} of carboxyl group of ASP269 is adopting the chair structure that leading to easy cleavage of the glycoside bond (During hydrolysis), the results of this study indicated that O_8 and O_{14} had maximum shift in B3LYP levels and played an important role in extra stability and the best interactions.
3. The charge value versus the isotropic and anisotropic values showed that charge Density was on O_8 and O_{14}.
4. The stability energy was reported and shown the most stability in B3LYP/6-31G level.
5. The dipole moment was observed that HF/3-21G was maximum.

3.1. Future objectives

1. A number of α-amylase structures are available therefore we can study the interesting results of this study on these structures. These structures including pig pancreatic amylase I [33,34], pig pancreatic amylase II [35,36], Aspergillus oryzae α-Amylases [37], barley α-amylase [38], Bacillus circulans cyclodextrin glycosyl transferase [39-41], Pseudoalteromonas haloplanctis α-amylase [42], and Bacillus stearo thermophilus "maltogenic" α-amylase [21]. In the overall fold of these structures, despite differences in their amino acid sequences, they have similar three dimensional structures, suggesting a similar catalytic mechanism. Therefore we can suggest the interesting results of this study on these structures. We suggest some of atoms that are similarly at nanotube-catalytic site of these alpha amylases and that

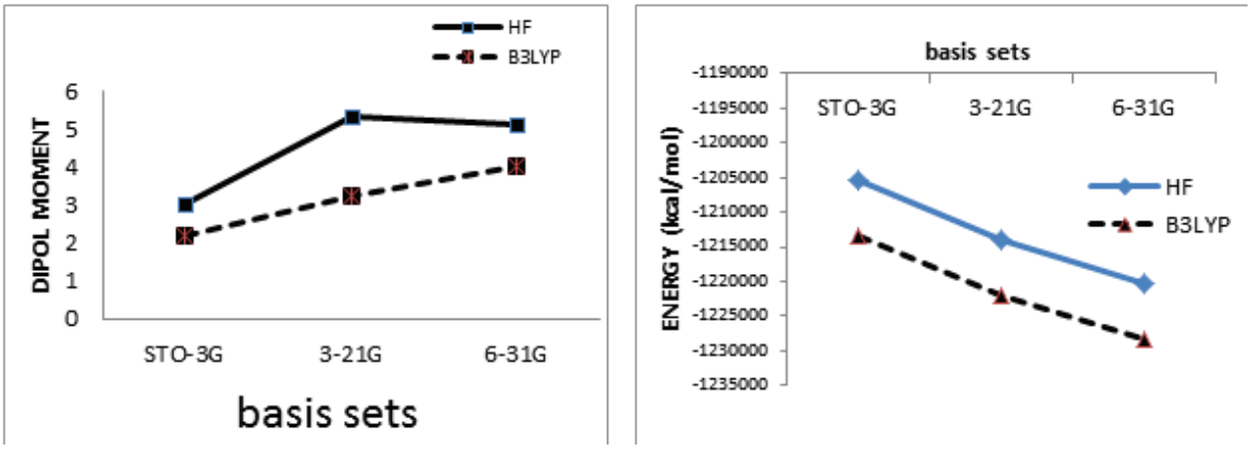


Figure 5: *Graphs of dipole moment (a) and stability energy (b) of nanotube-catalytic site in different basis sets using HF and B3LYP methods corresponding to Table 2.*

play an important role in extra stability.

2. These theoretical calculations have become a competitive alternative to successful assumptions and interpretation for nano-biochemical investigations.

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