MOLECULAR MODELLING OF SINGLE WALLED CARBON NANOTUBE WITH SINGLE STRAND DNA

Lalitha Jyotsna Nettem [1]*, N. Saritha[2], Vasudha Bakshi[3]

[1,3] Department of Biotechnology, Anurag Group of Institutions (Formerly Lalitha College of Pharmacy) Venkatapur (v), Ranga Reddy-500088, Telangana, India..

[2]Department of Chemistry, JNTUA, Kalikiri, Chittoor, Andhra Pradesh, India.

Corresponding author E-mail: lalitha.jyotsna@gmail.com

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ABSTRACT

Molecular modeling[1] includes wide range of molecular graphics and computational chemistry techniques used to build, display, manipulate, stimulate and analyze molecular structures. By calculating binding affinity the highest binding affinity molecule of single-walled carbon nanotubes (SWCNTs) with single strand DNA of 14bases[2] is identified. The diameter of the nanotubes was around 0.4, 0.7, 0.9, 1.1, 1.3, and 1.7 nm. The molecular dynamics and molecular mechanics of swcnt, ssDNA, and swcnt and ssDNA were calculated. In this study, the difference in force fields illustrated by comparing the calculated energies by using force fields such as AMBER ,MM+, and BIO+ .The single walled carbon nanotubes of chiral form with hand vector (8,2) of 0.7 nm showed good binding affinity with single strand DNA of 14 bases.

INTRODUCTION:

Molecular modelling [3] is a general term which covers a wide range of molecular graphics and computational chemistry [4] techniques used to build, display, manipulate, simulate, and analyze molecular structures, and to calculate properties of these structures. By calculating binding affinity the highest binding affinity molecule [5] of single walled carbon nanotube is identified. The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nanometric-level diameter [6-9]. Its structure, which is in the form of a hexagonal mesh, resembles a graphite sheet and it carries a carbon atom located on the vertex of each mesh. The sheet has rolled and its two edges have connected seamlessly [10-16]. There are three isomeric forms of single-walled nanotubes (SWCNTs): zigzag, arm-chair, and chiral nanotubes as enlisted in figure II. But, none of the developed methods of synthesis of such nanotubes provides pure, isomerically uniform products. Hence, the proposed methods available for separation of isomers [17] were based on their selective chemical functionalization. Single strand DNA have been shown to adsorb on single and bundled carbon nanotubes. Computational simulations suggested that a mixture of the carbon nanotubes can be separated with single strand DNA. The results depended on the

length of the SWCNTs. The adsorption improved with the increasing SWCNTS length and it was obscured, to a certain extent, by chain branching. The diameter of a carbon nanotube is another crucial factor [18–23].

A formal curvature of graphene plane into a single-walled carbon nanotube changed the properties of the molecular orbitals on both sides of the wall of the system to an extent depending on the degree of the curvature, that is, the diameter of the resulting nanotubes [24]. Originally, sp^2 hybridized carbon atoms of graphene structure changed their hybridization slightly towards sp^3. Hence, the electrical, emissive, and other properties of the nanotubes were modified. Obviously, the possibilities of interaction of the resulting outer molecular orbital with a single strand DNA were also perturbed. Additionally, three types of localizations of the carbon atoms of the nanotube walls in a manner providing isomerism might have subtly influenced the mode and energy of surface–sorbate interactions. Thus, in this work, the energy and structure of surface complexes of single-wall zigzag, armchair, and chiral carbon nanotubes of varying length and diameter with single strand DNA were simulated.

First, using the HyperChem 8.0 program the complex geometries optimized as enlisted in figure I. Energy minima were found by molecular dynamics (MD) calculations at 360 K (run time was 30 ps at step size of 0.001) and then by molecular mechanics (MM+) with RMS gradient of 0.001. Original parameters of the program were applied. The Gaussian 03 computations, using molecular mechanics (UFF) with four de-fault convergence criteria set in the program, were additionally performed. Computations were performed using commercial software package, HyperChem (HyperCube, FL). d(AT)14 oligonucleotides was obtained from the nucleic acid database, and was drawn in the vicinity to the SWNT. After geometry optimization was performed on the d (AT)14 DNA, energy minimization using Amber force field was conducted on the (AT)14-SWNT complex. The simulation was run for 30 psec until the conformation reaches equilibrium. In every case, computations were started using the HyperChem program (MD) with an initially optimized individual structure

of SWCNT and single strand DNA. This procedure was initiated by situating single strand DNA chains close to the nanotube surface but perpendicularly or at an angle to their long CNT axes. MD was applied for the first optimization run. During optimization, Single strand DNA could coil tightly around (and/or adhere along) CNT and the CNT–DNA complex was transferred through many local energetic minima, finally approaching the global minimum energy. Then the molecular mechanics MM+ method was used and a stationary point on the potential surface was found. Afterwards, the Gaussian 03 program (molecular mechanics UFF) was used to enhance the precision of the complex optimization process. This kind of computations was performed for zigzag, armchair, and chiral open-end single wall carbon nanotubes of the structure and the atomic composition specified in Table 1.

After a proper optimization of the CNT/DNA system geometry, the whole DNA chain should tightly adhere to the CNT surface independently of the DNA location on the CNT surface (coil and/or clip shape). Also, no part of the DNA chain could protrude from the CNT structure (as well as along the CNT axis and also perpendicular or at an angle to the CNT axis). In an optimized complex structure, the DNA could not self-cross. If one of those coincidences took place, optimization of the complex structure was repeated to avoid cases where the CNT surface was not fully covered by the DNA and the calculated complex formation energy would be significantly lowered (sometimes by over 20–30%). It was shown that the relation between the length of the CNT and the single strand DNA was not important. The single strand DNA could be much longer than the CNT and could tightly coil around the CNT several times or adhere to the CNT surface along the CNT axis, creating a kind of clip as shown below.

MATERIALS AND METHODS:

Softwares: Hyperchem:

Hyper Chem [25] is a versatile molecular modeler and editor and a powerful computational package. It offers many types of molecular and quantum mechanics calculations. For optimization of small molecules in solution and protein complex the

intra molecular energies of ligand-solvent and ligand protein will be calculated using molecular mechanics calculations of Hyperchem software enlisted in figure I.

Hyper Chem includes these functions:

1. Drawing molecules from atoms and converting them to three-dimensional (3D) models)
2. Constructing proteins and nucleic acids from standard residues.Using molecules from other sources; for example, Brookhaven Protein Data Bank (PDB) files.
3. Rearranging molecules by, for example, rotating and translating them changing display conditions, including stereo viewing, rendering models, and structural labels.
4. Setting up and directing chemical calculations, including molecular dynamics, by various molecular mechanical or abinitio or DFT or semi-empirical quantum mechanics methods
5. Determination of isotope effects in vibrational analysis calculations for semi-empirical and ab initio SCF methods. Graphing the results of chemical calculations and solvating molecules in a periodic box.

There are three steps in carrying out any quantum mechanical calculation in HyperChem 8.0 program .First, prepare a molecule with an appropriate starting geometry. Second, choose a calculation method and its associated options. Third, choose the type of calculation with the relevant options. The 14 base pairs (bp) DNA was constructed using the HyperChem polynucleotide builder and optimized with Amber96 force field using the Hyperchem 8 software. Computer simulation with Hyperchem 8 software was first carried to predict the stability of this system.

The 14 start codons of EFFPC1 were selected to build a single-stranded DNA (ssDNA) and combine with chiral form singlewalled carbon nanotube (SWCNT) with length 10nm. The computer simulation studies indicate that the ssDNA-SWCNT complex can form spontaneously and with a great stablility

through surface interaction as enlisted in figure III.

RESULTS:

The combination of CNTs with biologically important structures, such as DNA or polypeptides, is particularly intriguing since it opens the door to novel biotechnology and nanotechnology applications [26]. SWNTs have been considered as the leading candidate for nanodevice applications because of their one-dimensional electronic band structure, molecular size, biocompatibility and controllable property of electrical conductivity and reversible response to biochemical reagents [27].

Therefore, the interaction of biomolecules with SWNTs has generated a great deal of interest in the past few years [28]. SWNTs can be bind to the polymers and biological system such as DNA and carbohydrates. Computations were performed for six sets of open-end SWCNTs varying in their diameters, that is 0.4, 0.7, 0.9, 1.1, 1.3, and 1.7 nm. Each set contained three SWCNTsl. isomeric models, namely armchair (A), zigzag (Z), and chiral (C) nanotubes. Their structure and atomic composition is presented in the first column of Table 1. In the "Nanotube" column of the table the nanotube, diameter [nm], type of isomer (A – armchair, Z – zigzac, C – chiral), structure of nanotube (m,n), and number of the carbon and hydrogen atoms are given. In the DNA molecule column, subsequent values report energy [kcal/mole] of the SWCNT complex with a given DNA molecule, difference between energy of the complex and the sum of energies of the non-complexed partners, and the complex energy calculated for DNA molecule, respectively.

TABLE-1: Energies of the complex formation of ssDNA with the isomeric open end,
Single wall carbon nanotubes calculated with Hyper Chem 8.0 and Gaussian 03.

| NANOTUBE			DNA MOLECULE
Diameter	Isomeric form	Atomic composition	d(AT)$_{14}$
0.4	A	3,3 330C+12H	5225.73, -23.17,-0.26
	Z	5,0 276C+12H	2561.96, 52.02,2.00
	C	4,2 227C+13H	6698.32, 16.73,0.67
0.7	A	5,5 330C+20H	3499.25,25.43,1.59
	Z	9,0 432C+18H	4399.75, 30.03,1.88
	C	8,2 396C+20H	3943.48,25.44,1.59
0.9	A	7,7 467C+28H	3679.24,27.74,1.86
	Z	12,0 576C+24H	666037, 27.97,1.63
	C	8,5 436C+26H	3704.75,53.47,1.03
1.1	A	8,8 480C+32H	3327.61, 30.41,1.61
	Z	14,0 672C+28H	6803.62, 54.25, 2.15
	C	12,3 610C+30H	6205.52, 57.10,2.52
1.3	A	10,10 460C+40H	2550.44, 31.19,2.04
	Z	16,0 448C+32H	2868.48, 27.24, 1.61
	C	15,2 468C+34H	2944.08, 34.16, 2.17
1.7	A	13,1 3910C+52H	5046.19, 30.98, 1.74
	Z	22,0 1056C+44H	5555.13, 32.11,2.01
	C	18,6 826C+48H	4170.04, 32.03,2.15
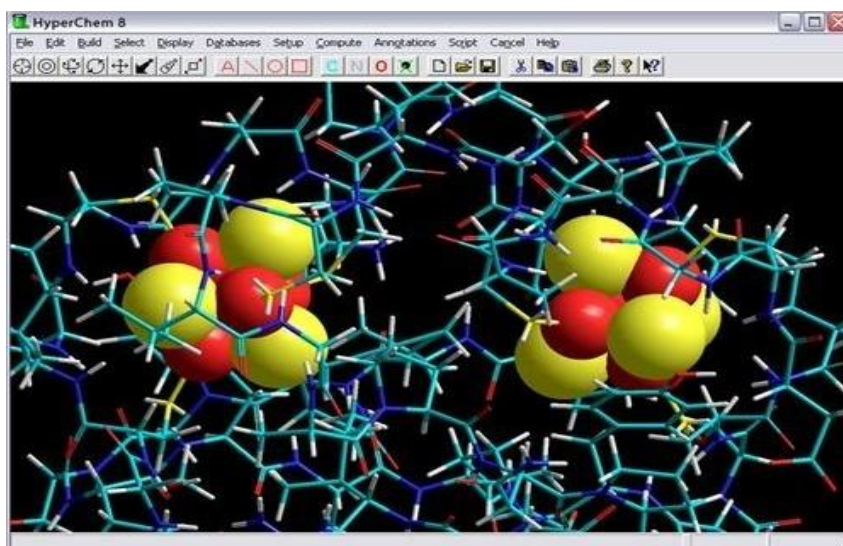
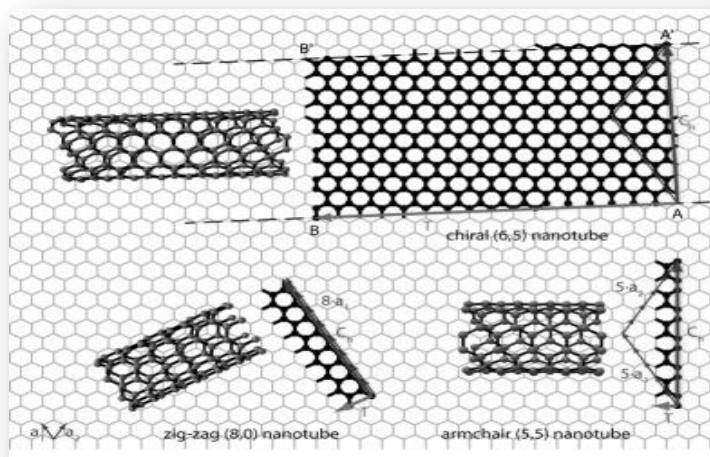**Figure I: Hyperchem Software**

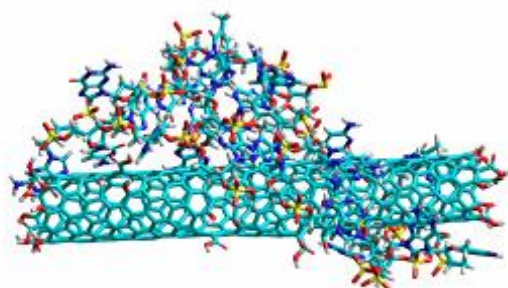**Figure 2: Images of single walled carbon nanotubes**

Figure 3: Complex of ssdna-swcnts

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