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PNA-CNT Interacting System: *In Silico* Investigation of Nanocarbon Sensors for PNA Detection

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ABSTRACT. Formation of peptide nuclei acid (PNA) interacting system with carbon nanotube (CNT) was investigated in this work employing the *in silico* computer-based calculation and simulation. The major problem of this work was to examine the sensor role of CNT nanocarbon for detection of PNA. First, the model of CNT was prepared according to semi-empirical approach for geometrical optimization and electronic property evaluation. The results indicated proper length size of CNT for contributing to interactions with other substances. Next, the model of PNA was prepared for running molecular docking simulation process. To this aim, the best conformational localization of CNT versus the already fixed PNA was explored to reach the most suitable PNA-CNT hybrid system. As a result, such hybrid formation was confirmed based on the obtained thermodynamic parameters proposing such CNT sensor for detection of PNA to be investigated by further works.

KEYWORDS. PNA; CNT; Nanocarbon; *In silico*; Semi-empirical; Computational.

INTRODUCTION. Several Application in biological living systems was indeed the most important expected mission from nanostructures, in which considerable efforts have been always dedicated to explore such features.[1-3] Although the starting point has been initiated by the innovation of carbon nanotube (CNT), but the future works indicated several other types of nanostructures applicable for various specific applications.[4-10] CNT itself has been the target of several research works of biological and non-biological topics from its first innovation by Iijima up to now.[11] Unique electronic properties and surface area made this pioneering nanocarbon material useful for verities of applications from inorganic media up to high-tech levels of life science.[12] Currently, CNT has been also the topic of considerable efforts for innovating novel applications for this unique material. Applications such as sensor have been seen provided with CNT for detection of several substances and also biological molecules or macromolecules.[13-15] To this point, such function was investigated in this work for detection of peptide nucleic acid (PNA) structure system. PNA is similar to DNA and RNA, in which the polymeric sequences of nucleobases are artificially synthesized at different scales and lengths.[16] Such PNA structures have been seen useful to put their function in biological living systems and therapies.[17] Characteristic features of PNA made them suitable materials to work in specified therapeutic purposes with higher binding affinity and chemical stability.[18] Sometimes, their recognition is not an easy task and considerable attempts should be put for recognition

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and separation process.[19] Therefore, designing a sensor could help for the purpose of facile detection of PNA in various media.

In this work, a hybrid system of PNA-CNT interacting system was investigated for such detection purpose of PNA based on nanocarbon sensor applications. The aim of this work was followed using *in silico* approach employing the computational methods for exploring molecular models of PNA-CNT hybrid system. The results were evaluated to be discussed to achieve a probable solution for the problem of PNA detection by using nanocarbon sensors.

METHODOLOGY. For this work, semi-empirical PM3 calculations were performed to optimize a representative (4,0) model of CNT using the Gaussian program to yield minimized energy structure.[20] Furthermore, infrared (IR) spectra was also evaluated for the optimized CNT and the same calculation level. Next, electronic properties of CNT were obtained by ZINDO calculations to show the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO) in addition to electrostatic potential (ESP) surface for the optimized CNT (Fig. 1). By doing such calculations, CNT was prepared for interacting with a representative PNA structure to make PNA-CNT hybrid system (Fig. 2). 3D molecular model of PNA was obtained for protein data bank (PDB ID: 1PUP) and it was prepared for further investigating by removal of water molecule. As a result, both models of PNA and CNT were prepared to be included in interacting complex formation process through molecular docking simulation using AutoDock program.[21] A grid box of 40×40×40 cubic size was created for 100 numbers of runs of genetic algorithm search of CNT conformational localization versus the rigid PNA target. Quantitative values in addition to qualitative representations were all summarized in Table 1 and Figs. 1 and 2 for further discussion to achieve the purpose of this work. It is worth to note that the results of this work were obtained based on the advantage of *in silico* computer-based approach to investigate materials at the lowest molecular systems, which are very much useful especially for complicated nono-bio systems.[22-33]

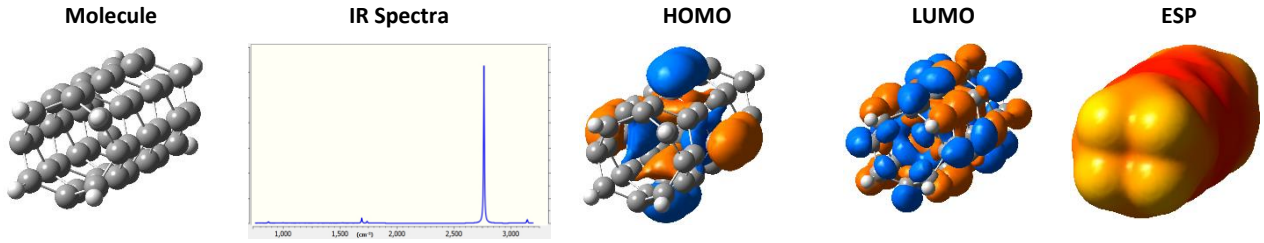

Fig. 1: Qualitative representations for the individual model of CNT.

RESULTS & DISCUSSION. Formation of PNA-CNT interacting system was investigated in this work employing *in silico* approach using semi-empirical calculations and molecular docking simulations. To this aim, a model of CNT (Fig. 1) was first prepared according to the optimization process using the semi-empirical method to reach the minimized energy geometers. Moreover, IR spectra was obtained for this optimized model at the same computational level. Indeed, electronic properties are arisen from structural basis of a chemical system, in which different structures could yield different electronic properties. This trend is very much important because of importance of such electronic system for assigning interacting properties for the investigated material. Such structural features and additional electronic properties could be discussed using the obtained IR spectra and other molecular orbital distribution patterns and ESP surface representation. As could be seen by panels of Fig. 1, such features were explored for the investigated CNT according to show electronic features of such unique material. It is important to mention here that the results were obtained by semi-empirical methodology of molecular calculations, in which they could be compared by other parallel results from different methods by a potential reader. Herein the results, the localization of HOMO and LUMO levels were seen at the surface of CNT with more localization at the center of tubular structure for HOMO pattern. This achievement could approve the earlier expectation about active surface of CNT for interacting with other substances. The other obtained qualitative

representation by ESP surface could also approve the achievement of proper interacting possibility for CNT with other substances. Further talking about such system could lead to another achievement that the size of CNT model was enough for this work by localizing the HOMO level at the middle of tubular length. In other words, this CNT could work as an active surface for contributing to interactions, in which the unique electronic properties could help for detection of other adsorbed substances by changes of such sensitive environment at the molecular site. It is somehow a kind of molecular architecture.

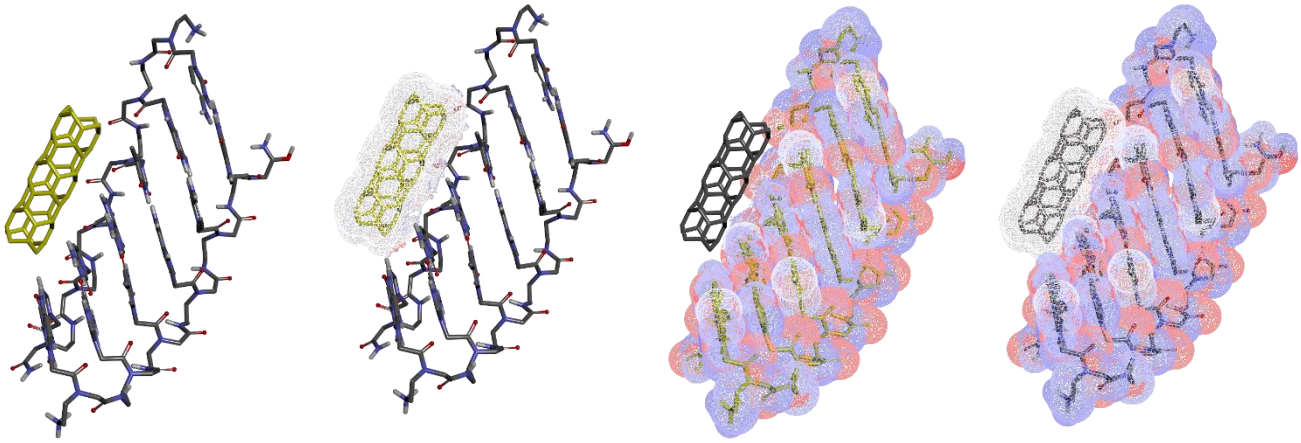

Fig. 2: Qualitative representation of PNA-CNT hybrid with various exhibition of van der Waals radii.

To create hybrid PNA-CNT interacting system (Fig. 2), molecular docking simulation was performed to achieve the best conformational localization of CNT versus the already fixed PNA. The model of PNA was a double strand with seven nucleobase in each strand. It was expected that the CNT could penetrate inside the two strands of PNA; but it was located at the outer side of one of strands towards peptide linkers of PNA sequence. This result was very much interesting to show an additional role for the peptide linkers for preparing detection sites besides their initial role of bases linking. The value of binding energy (BE) was obtained -8.45 kcal/mol showing almost a strong interaction between CNT and PNA. Furthermore, the value of 33.50 Å for RMSD could show that the CNT was located at the proper position by enough conformational change for the purpose. Other results of Table 1 showed that the shortest length of interaction between CNT and PNA was 2.85 Å as a good intermolecular distance (ID) for non-covalent interactions. Negative value of free energy (A) and positive value of entropy (S) at 298.15 K both approved the formation possibility of such PNA-CNT hybrid system. In this case, such hybrid formation could be easily measured by excess concentration of remained CNT in the environment. The value of 645.26 nM for inhibition constant (KI) showed that all concentration of CNT should be sued for PNA-CNT hybrid formation in a ratio of 1:1. Therefore, it is a good choice to detect PNA according to measurement of the remained CNT.

Table 1: Molecular docking results for PNA-CNT hybrid.

BE kcal/mol	**RMSD** Å	**KI** nM	**ID** Å	**A** kcal/mol	**S** kcal/mol/K
-8.45	33.50	645.26	2.85	-2736.91	9.15

CONCLUSION. In this work, formation of hybrid of PNA-CNT interacting system was investigated employing the *in silico* computer-based approach methodologies. The non-covalent interacting system of PNA and CNT was created by performing molecular docking simulation, which showed the best conformational localization of CNT versus the peptide linker of PNA. The value of binding energy was suitable enough for a strong non-covalent interacting system in addition to reasonable interacting distance of two molecular counterparts of hybrid. Other obtained values all approved that such formation could be obtained, in which the inhibition constant indicated that the excess concentration of CNT after hybridization should be traceless amount. As a final remark, such CNT sensor could be proposed for

detection of PNA to be investigated by further research works.

DISCLOSURE STATEMENT. The author(s) did not report any potential conflict of interest.

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