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Finding the best angle, between carbon nanotubes and four groups of antibiotics, using computational methods

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ABSTRACT: In this work, the first in the world of science, the focus was on the best angle of connection between carbon nanotubes and the most widely used group of antibiotics. While having the highest stability, in terms of energy, we have the best angle of to connect to the in vivo delivery of intraoperative antibiotic binding with carbon nanotubes not lost. It will never work in the world of science. Connecting the carbon nanotube and antibiotics precise targeting to sites of infection within the body and a much lower dose of antibiotics is needed. Because of the sensitive nature of the initiative was measured 4 times per connection to ensure the accuracy of the results is sufficient and also because of the novelty of attitude associated with that particular phase diagrams were drawn at each stage to witness the results of the arguments made. In this work, the four antibiotics: penicillin, tetracycline, Ampicillin and gentamicin were used. Appropriate connect between carbon nanotubes and antibiotics, respectively Carbon nanotubes and penicillin 177°.Carbon nanotubes and Tetracycline 201°. Carbon nanotubes and Ampicillin 172° and Gentamicin and Carbon nanotubes 189°.

Keywords: *Antibiotic; Bond energy; Carbon nanotubes; Connection angles; Computational method*

INTRODUCTION

Origin of the word antibiotic means anti-life, anti Bios taken (Lindemeyer, *et al.*, 1962). Two researchers in 1877 AD, the effect of bacteria on the anthrax bacterium (Bacillus anthracis Anthrax is caused by Tremblay) observed and the term anti Bios as used (Higgens and Kastner, 1968). Then these bacteria of effective substance called antibiotic. Antibiotics are chemical substances produced by microorganisms (bacteria, fungi, molds), or semi-synthetic production and caused interruption of critical phenomena in other organisms, ie, microorganisms (bacteria, fungi, parasites, viruses) or aimed at cancer cells (Benveniste and Davies, 1971). The origin of the three categories: natural source, origin semi-synthetic and fully synthetic aimed division. Of antibiotics are often linked to one of the following combinations:

1. Polypeptide and protein: peptide structures are some

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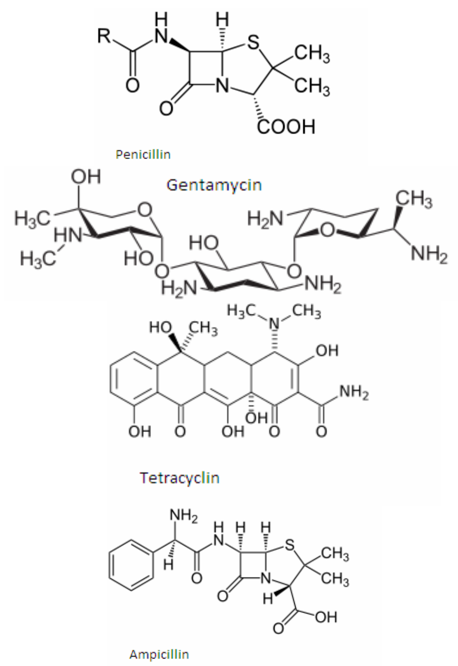

Scheme 1. The sturctures of four antibiotics: Penicillin, Tetracycline, Ampicillin and Gentamicin

antibiotics such as penicillin and ampicillin,

2. Carbohydrates: Sugars and derivatives of certain antibiotics such as gentamicin,

3. Polycyclic: Some other antibiotics are derivatives of naphthalene and polycyclic such as Tetracycline (Pedersen, *et al.*, 1972).

There are some unique characteristics of carbon nanotubes make them an ideal nanostructures is suitable for many biomedical applications (Pantarotto, *et al.*, 2004). Carbon nanotubes of carbon nanostructures Due to the hollow structure and small (smaller than red blood cells) (Ke and Qiao, 2007), specific roles in the biomedical field such as drug delivery to target cells (Liu, *et al.*, 2007), Blood Glucose Biosensor recognize (Liu, *et al.*, 2008) and destroy cancer cells (Wu, *et al.*, 2008), tissue engineering and so on (Podesta, *et al.*, 2009). Recent studies have shown that carbon nanotubes can be used for biological targets, such as protein crystallization, and the construction of bioreactors and biosensors used (Kostarelos and Bianco, 2009, Bhirde, *et al.*, 2009).

Liu and colleagues drug Doxorubicin (DOX) for the treatment of cancer into pre-defined groups functionalized nano tubes which have been entered, The results showed that the drug is complexed with carbon nanotubes (DOX-SWCNT) high stability in aqueous media at physiological pH (Liu, *et al.*, 2009). Tabakman and colleagues injected single-walled nanotubes by controlling the concentration liver cancer tumors in rabbits, and then placed the radio frequency. After 48 hours the tumor was removed (Liu, *et al.*, 2009). Takai and colleagues developed a sensitive Biosensor for measuring and identifying bacteria based selective field-effect transistor a network of single-walled carbon nanotubes on a conducting channel are used (Takei, *et al.*, 2010), Researchers properties of carbon nanotube biosensors were used to measure glucose (Jin, *et al.*, 2010), These sensors are easily within living tissue using a laser capable of quickly display blood glucose levels are high precision measurement (Liu, *et al.*, 2013), Kim and colleagues used carbon nanotubes as a navigator and the drug delivery used and the results were reported (Kim, *et al.*, 2013). Since most research has been conducted in connection with the stability problem encountered seemed to do the necessary research.

COMPUTATIONAL METHOD

In this paper, we only discuss the simulation work, which is expressed exclusively in the simulation of interconnects, carbon nanotubes and antibiotics. At the beginning of each antibiotic using Chem Draw software is plotted on the three dimensional Chew3D programs were presented (Figs. 1-4). Next, single-walled nanotubes (4.7), which is used in the project also displayed on Chem3D (Fig. 5). In the next step, every single antibiotic with carbon nanotubes on a program Chem3D, under different angles were connected again on a program ChemDraw was implemented and the connection angles were recorded. For each combination of carbon nanotubes and antibiotics "6" different angles of binding was checked. The next step is to ensure that the connection is one of the 24 states on Hyperchem program was implemented, so the connection was reliable (Figs. 6-9). Finally, using the Gaussian and command HF/3-21g for each of the twenty-four states Energy Optimization and Dipolemoment calculated and with the program Gaussian for each of these cases taken NMR.

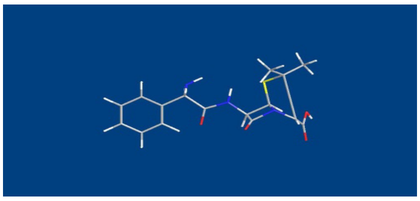

Fig. 1. Penicilin

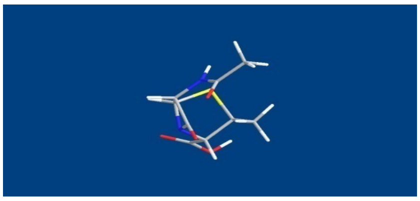

Fig. 2. Ampicilin

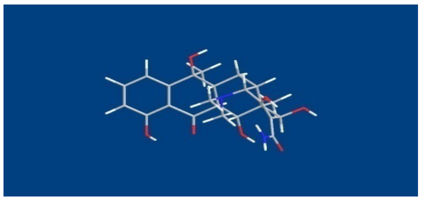

Fig. 3. Gentamicin

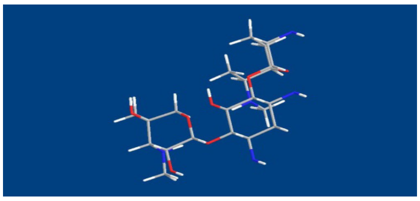

Fig. 4. Tetracycline

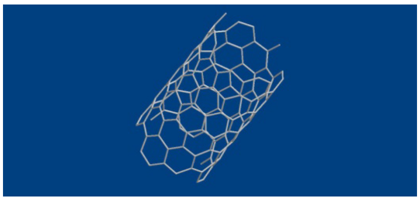

Fig. 5. Carbon nanotubes (4.7)

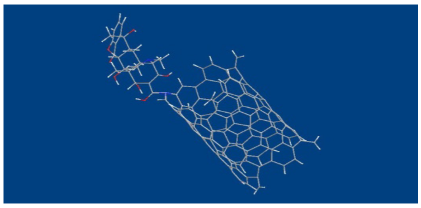

Fig. 6. Tetracycline + Carbon nanotube

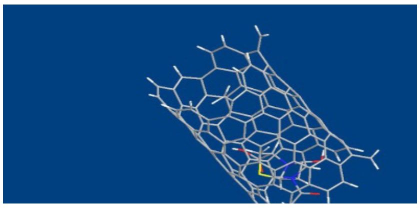

Fig. 7. Penicilin + Carbon nanotube

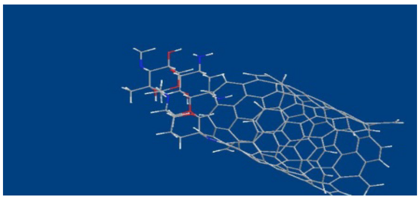

Fig. 8. Gentamicin + Carbon nanotube

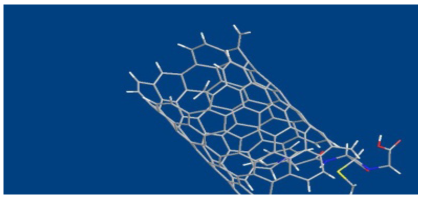

Fig. 9. Ampicilin + Carbon nanotube

RESULTS AND DISCUSSION

Below the results from NMR, H-1 and NMR, C-13 for each of the twenty-four states shown (Figs. 10-15): For connection between carbon nanotubes and ampicillin at six angles: 71,120,177,189,223,301 For connection between carbon nanotubes and penicillin at six angles: 71,120,177,189,223,301 For connection between carbon nanotubes and Gentamicin at six angles: 71,120,177,189,223,301

For connection between carbon nanotube and Tetracyclin at six angles: 71,120,177,189,223,301

As it is clearly visible on curves by changing the connection angles are different forms of registered NMR and Chemical shifts are different for each angle control connection. Also see the following links taken out NMR and angles are (Its changes are obvious the angles connection to the average NMR). Again due to the increasing volume of contents from any of a variety of NMR are only two cases were brought. Survey graphs show logical relation between the energy and the chemical shifts, Much less influence adjacent of the nucleus of studied by NMR The average chemical shifts down and the cause of the link is stable. So the binding energy levels stable, the average chemical shift is related to the link below. All information obtained

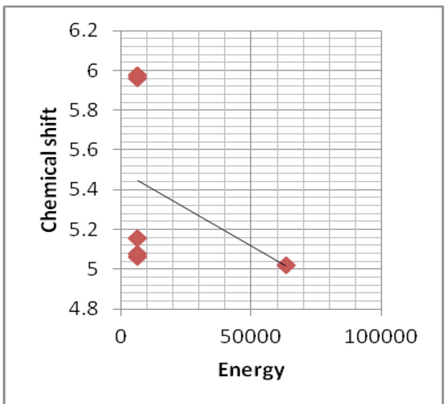

Fig. 10. NMR C-13 between Carbon Nanotube + Penicilin

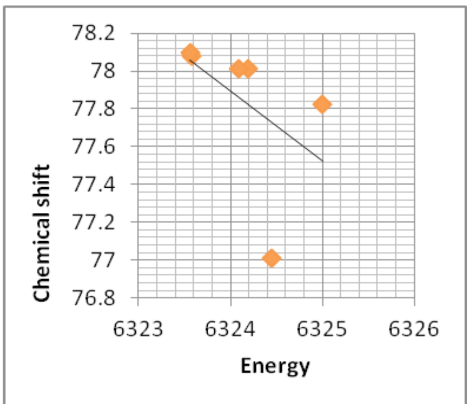

Fig. 11. NMR H-1 between Carbon Nanotube + Penicilin

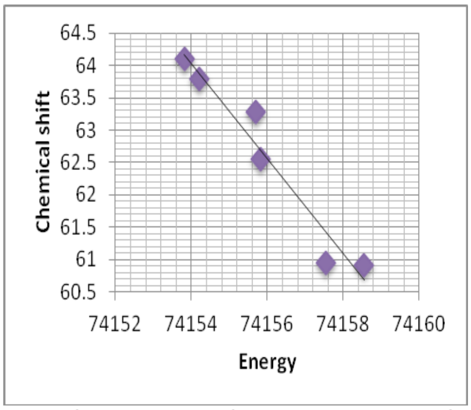

Fig. 12. NMR C-13 between Carbon Nanotube + Gentamicin

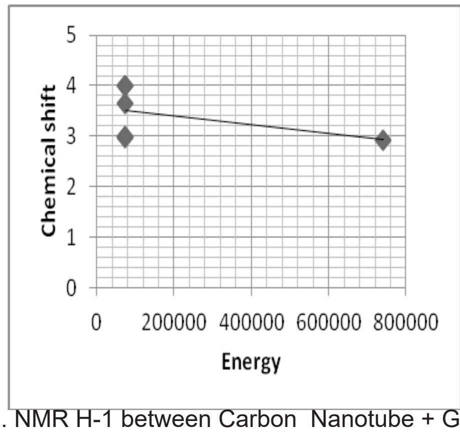

Fig. 13. NMR H-1 between Carbon Nanotube + Gentamicin

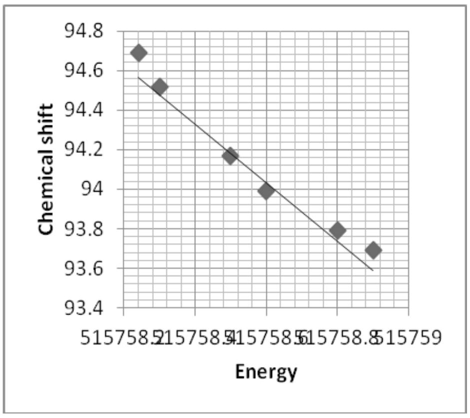

Fig. 14. NMR C-13 between Carbon Nanotube + Ampicilin

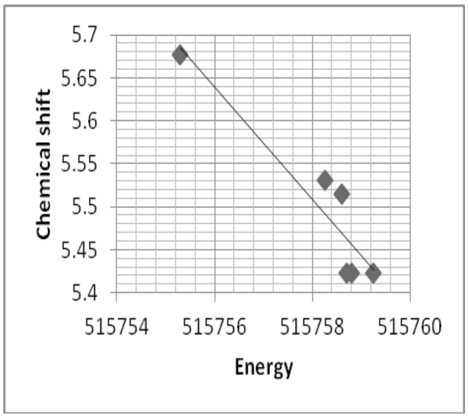

Fig. 15. NMR H-1 between Carbon Nanotube + Ampicilin

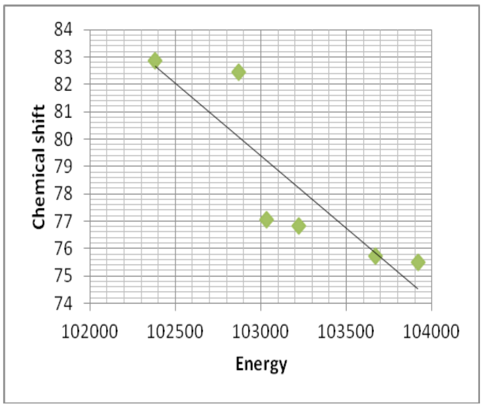

Fig. 16. NMR C-13 between Carbon Nanotube + Tetracyclin

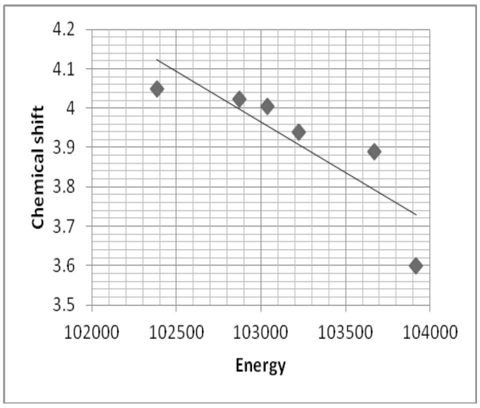

Fig. 17. NMR H-1 between Carbon Nanotube + Tetracyclin

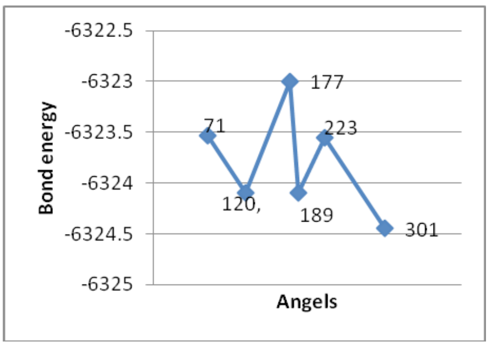

Fig. 18. Communication between link energy and conect angle in the conected between Nanotube + Gentamicin

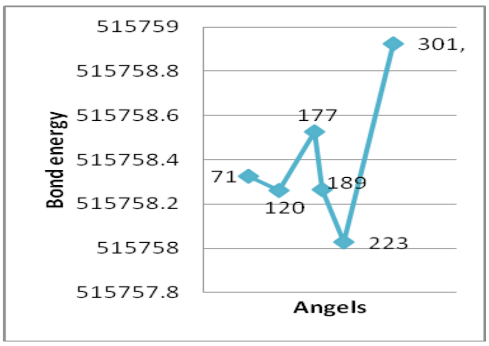

Fig. 19. Communication between link energy and conect angle in the conected between Nanotube + Tetracyclin

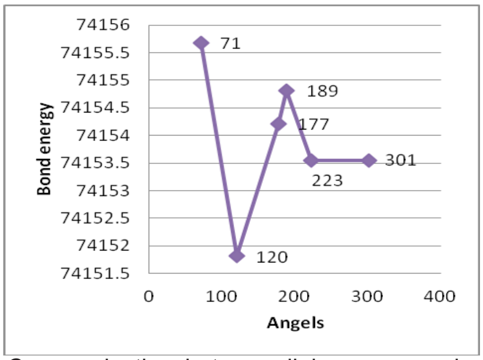

Fig. 20. Communication between link energy and conect angle in the conected between Nanotube + Penicilin

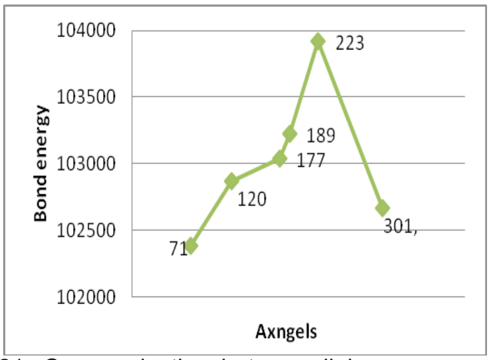

Fig. 21. Communication between link energy and conect angle in the conected between Nanotube + Ampicilin

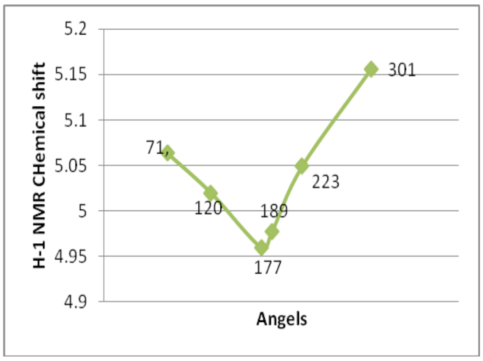

Fig. 22. Communication between chemical shift NMR H-1 and conect angle the conected between nanotube + Gentamicin

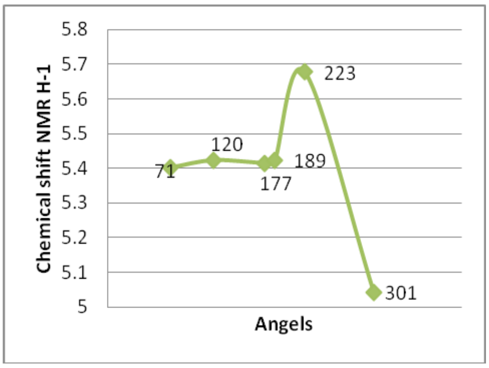

Fig. 23. Communication between chemical shift NMR H-1 and conect angle and conect angle in the conected between nanotube + Tetracyclin

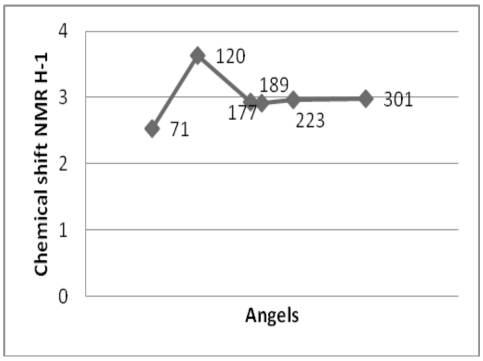

Fig. 24. Communication between chemical shift NMR H-1 and connect angel in conected between nanotube + Penicillin

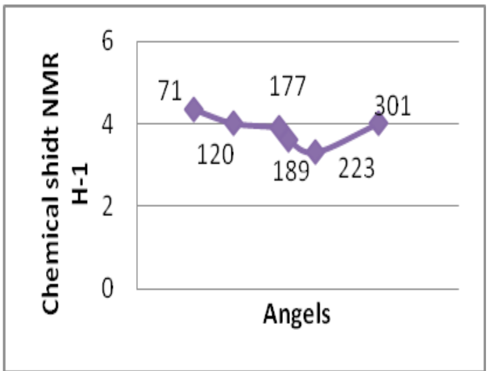

Fig. 25. Communication between chemical shift NMR H-1 and connect angel in the conected between nanotube + Ampicillin

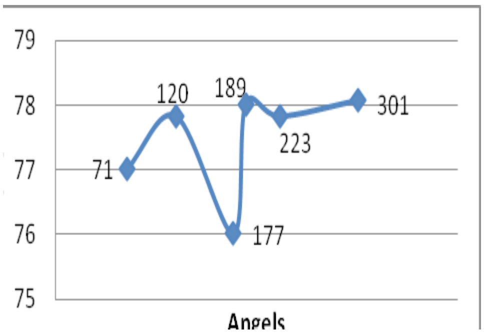

Fig. 26. Communication between chemical shift NMR C-13 and connect angle in the connected between nanotube + Gentamicin

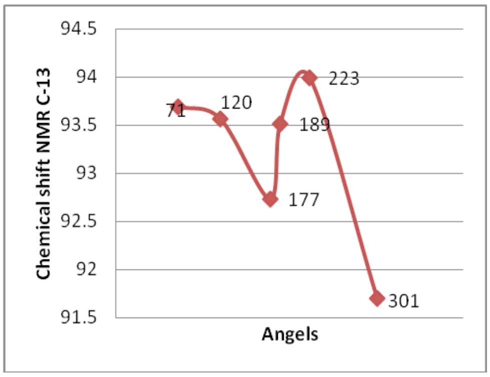

Fig. 27. Communication between chemical shift NMR C-13 connect angle in the connected between nanotube + Tetracyclin

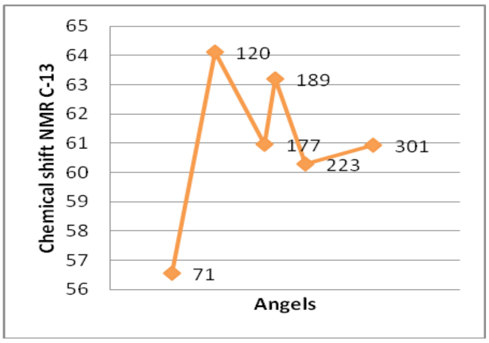

Fig. 28. Communication between chemical shift NMR C-13 andconnect angle in the connected between nanotube + Penicillin

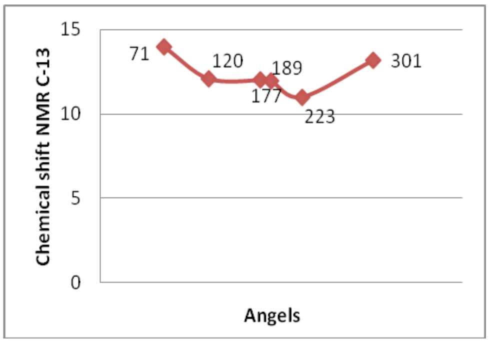

Fig. 29. Communication between chemical shift NMR C-13 and connect angle in the connected between nanotube + Ampicillin

Collected in Tables to find the best angle, are shown. In all cases shown the link between carbon nanotubes and any antibiotics quite a difference by changing the angle of the connection are in NMR H-1 and C-13. The difference between the numbers given in the Tables, Can be compared in terms of the numbers of the energy levels to achieve the best angle connector. It is also worth noting that the linear regression indicates significant differences within and between the impact angle and the surface binding energy is clearly visible in the graphs, Check the connection diagrams contribute to achieve the best angle is because we have a much lower energy barrier, The chemical shifts will be lower and the charts will be located in the lower part and thus it could be argued The connection angle is located at the lowest part of the graph best angle of connection between carbon nanotubes and antibiotics (Tables 1-4).

Table 1. Different angles and energies between Tetracyclin and Carbon nanotube

71	6323.53
120	6324.00
177	6324.44
189	6324.11
223	6323.25
301	6323.00

Table 2. Different angles and energies between Ampicilin and Carbon nanotube

71	103035.8
120	103221.1
177	103669.6
189	103917.7
223	102382.2
301	102872.5

Table 3. Different angles and energies between Gentamicin and Carbon nanotube

71	515758.66
120	515758.26
177	515758.07
189	515758.56
223	515758.47
301	515758.86

Table 4. Different angles and energies between Penicilin and Carbon nanotube

71	74151.27
120	74154.82
177	74154.22
189	74153.69
223	74153.11
301	74151.78

Looking at the Tables of the best angel of connection for:
For Tetracyclin and Carbon nanotube is 301°
For Ampicilin and Carbon nanotube is 223°
For Penicilin and Carbon nanotube is 71°
For Gentamicin and Carbon nanotube is 177°

CONCLUSIONS

With the best angle of connection for each antibiotic with carbon nanotubes could be used to provide a Combination of antibiotics and carbon nanotubes. Whatever is selected will cause more right angle of connector that links greater stability in vivo, and thus the delivery of carbon nanotubes have been used as carriers Can transmit larger amounts of the drug to the desired location with a smaller amount of the drug after its effective dose applied to the desired location. Use the link could be thousands of times lower dose of the drug (Campagnolo, *et al.*, 2013). Carbon nanotubes could be precisely using antibiotics to the site of infection transmission and having the energy level of the bonding angle of in the pharmaceutical industry is very practical (Rastogi, *et al.*, 2014).

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