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***Research Article***

# COMPARING THE ISOTHERM OF STEROIDAL DRUG DEXAMETHASONE AND NON-STEROIDAL DRUG CIMETIDINE BY USING MULTI-WALLED CARBON NANOTUBES AND SINGLE-WALLED NANOTUBES

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## ABSTRACT
In this laboratory study, adsorption isotherms of the steroidal drug dexamethasone and non-steroidal drug cimetidine have been studied by using single-walled and multi-walled carbon nanotubes by use of a spectrophotometer. Absorption at several different density, have been studied and calculated and its graphs have been drawn. Results obtained by Temkin, Frundlich and Langmuir equations were studied.

***Keywords:*** *Multi-walled Carbon Nanotubes, Single-walled Carbon Nanotubes, Isotherms, Ranitidine*

## INTRODUCTION
Nano is a Greek word that means small, and use to determine the value of one- billionth or $10^{-9}$ of a quantity. Because an atom is approximately "10 nm, this term is applied to the general study of the atomic and molecular particles. Nano science and related sciences are not new, because hundreds of years the chemists use of Nano science techniques in their own work that is not unlike the Nano modern techniques. Colorful windows of medieval churches, swords found in Muslim lands excavations all suggest that Man for long time has been used some techniques of this technology to optimize the processes and manufacturing high-quality objects But just because of low development of technology and lack of modern facilities such as atomic force microscope, scanning tunneling microscope, etc. did not determine any specific area for this technology.

### *History of Nanotechnology*

For the first time, Nobel Prize-winning physicist Richard Feynman raised Nano science potential in a startling speech called "bottom there are many rooms". Feynman insisted that scientists begin to build devices that are necessary to work at the atomic scale. It remains blacked until Eric Drexler (MIT Graduate Student) heard Feynman voice and created a framework for the study of "devices capable of moving molecular objects and their place with atomic precision", that in September 1981 offered it in an article entitled "Protein provides a way to molecular mass production ". Drexler followed it with his book entitled "Engines of Creation" and continued development of nanotechnology concept as a scientific endeavor.

### *Nanotechnology Developments*

Nanotechnology is an important area in science and technology that attract the attention of countries, firms, educational and research institutions and researchers in recent years. Presence in this field is inevitable for countries and it is also necessary for our country but in this area timely and accurate decisions are necessary and one of the main requirements is the formation of innovation network in the selected axis. Developing and implementing a comprehensive and providential plan and cross-sectorial coordinating resolver entity is also one of the conditions for success in this field (John, 2011).

### *Allotropes of Carbon*

Until 1980, three allotrope of Carbon (non-crystalline) as diamond, graphite and amorphous carbon were known, but today we know full family of other forms of carbon (Figure 1-1).

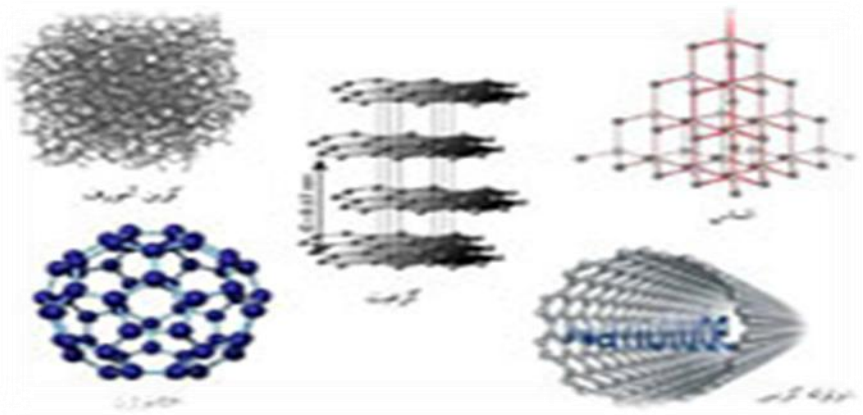

**Figure 1-1: different allotropes of carbon**

The first allotrope of carbon that was discovered in 1985 was called Buck Minster fullerene which is named in other names Bucky Ball and fullerene. Fullerenes are spherical molecules of carbon that due to the beautiful shape and amazing properties, have drawn the attention of many scientists. In 1991 a scientist named Sumio Ijima, quite by chance, discover and produce another structure of carbon that has unique properties. He initially thought that this structure is a fullerene which is stretched in one direction. But later he realized that this structure has different properties of fullerenes and that's why it's called a carbon nanotube.

***Types of Carbon Annotates***

There are two types of carbon nanotubes: single-walled nanotubes and multi-walled (Langmuir, 1918). Single-walled carbon nanotube is formed of a graphite barrel wall diameter of 1 to 2 nm. Now, if the single-wall nanotubes place inside each other with a distance of 3-4 nm and outer cylinders diameter become larger, a multi-wall carbon nanotube is formed. Outer diameter of Multi-wall nanotube is from 2 to 25 nm and the inner diameter of about 1 to 8 nm. The average length of the nanotubes can be up to several microns.

***Steroids***

Steroids are modified terpenes which are made from squalen non-cyclic hydrocarbon in the living organism. The exact path of this conversion is wonderful, long and complex, but its key steps have been elucidated in Institute of Conrad Black and John Konfort who catch Nobel Prize for their works. Biosynthesis of steroids begins by enzyme epoxidation of squalen and squalen oxide production that by making ring and a marvelous collection of nine carbocation reaction, squalen in the presence of acid catalysts leads to lanesterol. In the next step, Lanesterol break down to the cholesterol by other enzymes. The produced cholesterol is converted into a series of different steroids by various enzymes.

***Dexamethasone***

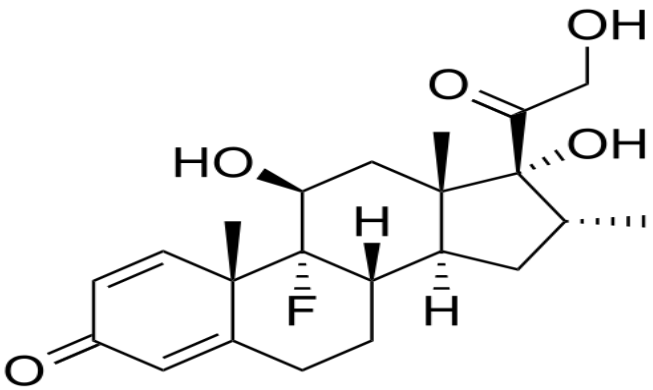


**Figure 2.1: Molecular structure of dexamethasone**

***Explanations***

Corticosteroids like dexamethasone are drugs that their action is similar to the action of secreted hormone by the human adrenal cortex and often used in cases that the body is unable to manufacture enough of these hormones. Also these drugs are used in cases of inflammation (swelling, redness, pain), treatment of special forms of arteritis, skin diseases, hematologic, renal, thyroid, bowel, severe allergies and asthma and … . This drug is also used to treat especial kinds of cancers.

In high positional density, Corticosteroids have a direct effect on membrane. Corticosteroids reduce cell and fibrin exudate and tissue infiltration. Preventing the formation of collagen and connective tissue, delaying in production of epithelial cells, reduce the formation of new blood vessels after inflammation and reduce the permeability of the swell capillaries, are the other effects of these drugs (Dexamethasone).

***Non-steroidal***

Non-steroidal anti-inflammatory drugs (NSAID) are one of the most commonly used medicines. These drugs inhibit cyclooxygenase and have three important properties such as reducing inflammation, analgesic and febrifuge. This class of drugs has anti-inflammatory effects at high doses. NSAID are so unique because they are non-addictive and do not cause addiction. Famotidine, omeprazole, ranitidine and cimetidine are examples of these drugs.

Non-steroidal anti-inflammatory drugs in terms of matter and the basic structure is divided into the following groups:

1- Salicylates
2- Alcanoic acids
3- Derivatives of propionic acid
4- Other groups

***Cimetidine***

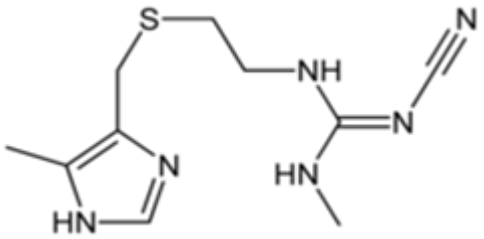


**Figure 2-1: Molecular structure of cimetidine**

***Explanations***

Cimetidine is used in the short term treatment of active duodenal ulcers or active and benign gastric ulcers, pathologic of excessive secretion of stomach acid, such as zollinger-ellison syndrome, Gastro esophageal reflux or other cases that the reduction of stomach acid is helpful to them, such as gastrointestinal surgery.

These drugs inhibit basic secretion of gastric acid and Nocturnal secretion of it through competition with histamine in the surface of H2 receptors of the wall cell. This drug inhibits gastric secretion stimulated by food, caffeine, insulin, histamine, Betazole and pentagastrin. Cimetidine may increase the resistance of gastric mucosal and its recovery. Cimetidine absorption is reduced in the presence of antacids. [3]

***Adsorptions***

In the adsorption process, a component of the gas or liquid phase is transferred to a solid surface. The term adsorption is used to describe the fact that the density of adsorbed molecules on solid surfaces is greater than the gas phase or solution. Adsorbed on a solid surface is due to gravity of atoms or molecules at that solid surface. In process of adsorption, several forces such as both physical and chemical are effective and its amount depends on the nature of the absorbed material and adsorbent material and because of that it can be separated a substance in a mixture.

There are two main mechanisms for adsorption:

(1) Physical Absorption
(2) Chemical Absorption

***Isotherms of Adsorption***

In a two-component system consisting of adsorbents and dissolved, a diagram of the dissolved concentration on solid phase $q_e$ (mg / g) versus the dissolved concentration in a solution $C_e$ (mg / L) at equilibrium, is expressed an adsorption isotherm. Adsorption isotherms are considered to describe adsorption capacity in order to facilitate the assessment of the feasibility of the process for the application and are useful for the analysis and design of adsorption systems.

***Langmuir Isotherm***

This adsorption model that is the most commonly used is described by the following equation (Langmuir, 1918):

(1-3) q=(k_a q_m C)/(1+k_a C)

Here q is the dissolved value of adsorption (mg / g) and Ceq is dissolved concentration in a solution at the equilibrium moment (MgL-1). qm and Ka are Langmuir constants which respectively indicate the maximum adsorption capacity and energy of adsorption. Linear model is obtained by rearrangement of Equation 1:

(2-3) 1/q_m =1/(K_a q_m C_e )+1/q_m

Therefore, the graph of q/1 versus Ce/1, will be a straight line with a slope of qm Ce /1 and intercept qm/1.

Langmuir model for monolayer adsorption onto the adsorbent material surface has valid limited and same absorption sites. Essential characteristic of the Langmuir Is defined as follows by RL constant which is known as equilibrium parameter.

(3-3) RL=1/( 〖1+(k_a c_0〗

ka is the Langmuir constant and C0 is initial concentration (mg / L). Value of RL indicates the type of isotherm, Isotherm is irreversible if RL = 0, RL <1> 0 favorable isotherm, RL = 1 linear isotherm and if RL> 1 the isotherm is unfavorable.

***Frundlich Isotherm***

Frundlich isotherm is an empirical equation for the adsorption of ions on the surface of heterogeneous with multi-layered adsorption and the dissolved amount increases indefinitely with increasing the concentration. Frundlich adsorption isotherms are described by the following equation (Abdulrahman *et al.*, 2008):

(4-3) $$q = KFCeq^{\frac{1}{n}}$$

In this equation q is the amount of adsorbed material ($mgg^{-1}$) and Ce is adsorb concentration in solution at the equilibrium moment 1/ n and $k_f$ are Frundlich constants that respectively are the adsorption intensity and the adsorption capacity. The line form of equation 4 is as follows:

(5-3) $$\ln q_e = \ln K_f + \frac{1}{n}\ln C_e$$

The ($lnq_e$) diagram by ($lnC_e$) will be a straight line that its slope is 1 / n and its intercept is $lnk_f$ .

Frundlich model is built based on monolayer adsorption on heterogeneous adsorption sites with Non-uniform and unequal energy. In the Freundlich isotherm when $K_F$ increases the absorption capacity of absorbent increases to absorb the desired material, also the value of n between 1 and 0/1 indicates perfect absorption process. If the value of n is closer to 1, being heterogeneous of the level is less important and if it is closer to 0/1 is more important.

***Temkin Isotherm***

Temkin isotherm contains a factor that shows interactions between the adsorbent and the adsorb particles clearly. Temkin isotherms obtained in this way (Zahangir *et al.*, 2008):

$$q_e = \frac{RT}{b}\ln(AC_e) \quad (6\text{-}3)$$

Considering B = RT / b, a linear form of Temkin isotherms will be as follows:

$$q_e = B_1 \ln A + B_1 \ln C_e \quad (7\text{-}3)$$

Here A [28] in (L / mg) is equal to the link constant associated with the maximum binding energy, B (without unit) is Temkin isotherm Constance and b (J / mol) is proportional to the heat of adsorption. Adsorption data could be derived from the equation.

## MATERIALS AND METHODS

100 ppm solution of steroidal drug dexamethasone and non-steroidal cimetidine produced and its Maximum wavelength ($\lambda_{max}$ ) determined by the UV-VIS set. Then we take the adsorption rate in several different concentration of the solution. Then add 0/01 grams of carbon nanotube and put on a magnetic stirrer and then measure the absorbance at the initial concentration by the UV-VIS. Then calculate the adsorption isotherms and draw the diagrams by using EXCEL software.

***Drawing Diagrams and Calculating Parameters***

***Dexamethasone***

**Table 1: Calculating parameters of adsorption isotherms of Langmuir, Frundlich and Temkin for dexamethasone adsorption on multi-walled carbon nanotubes**

| Frundlich | Langmuir | Temkin |
|---|---|---|
| $R^2$= 0.999 | $R^2$= 0.9724 | $R^2$= 0.9872 |
| n = 1.34 | Qm(mg/g) =72.99 | B = 13.45 |
| $K_f$(mg/g) =4.92 | $K_a$(L/mg) =.058 | A = $e^{-0.36}$ |
| ------- | $R_L$=0.54 | b= 190.42 |

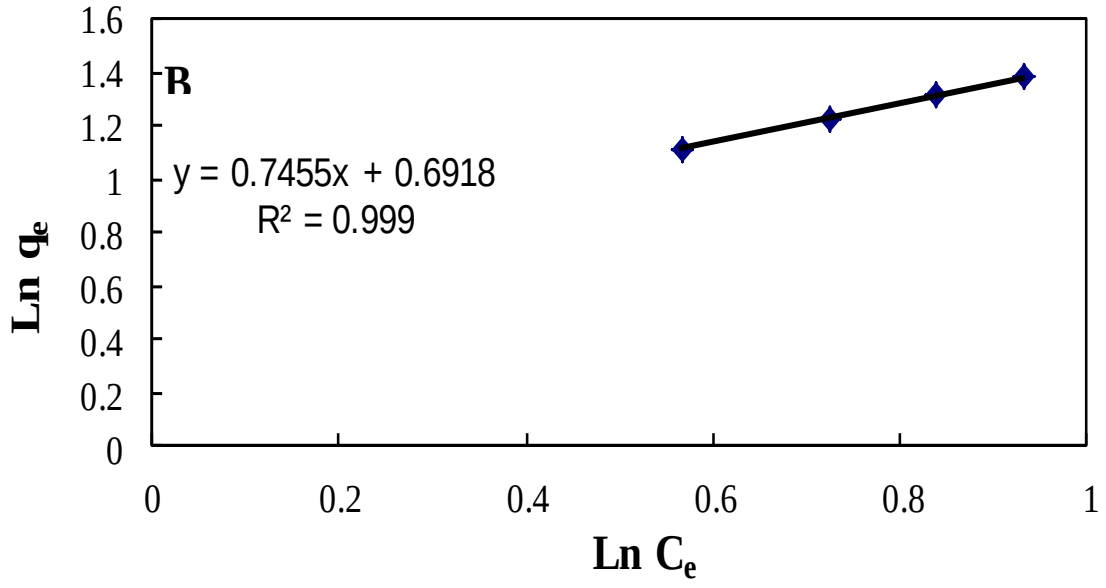


**Figure 1: Diagram of dexamethasone adsorption based on the Frundlich adsorption model**

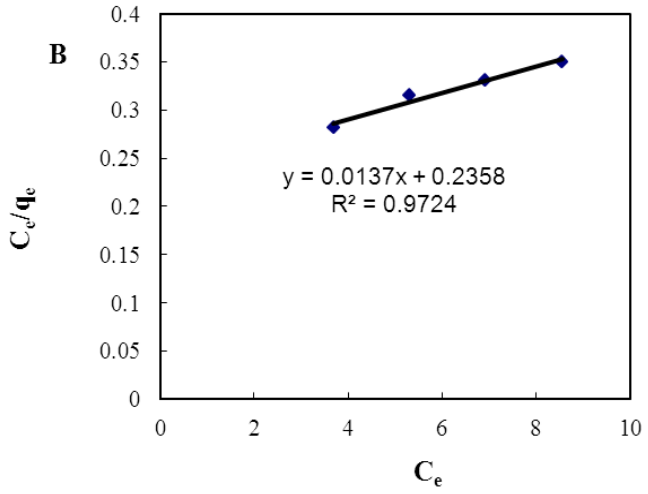


**Figure 2: Diagram of dexamethasone adsorption based on the Langmuir adsorption model**

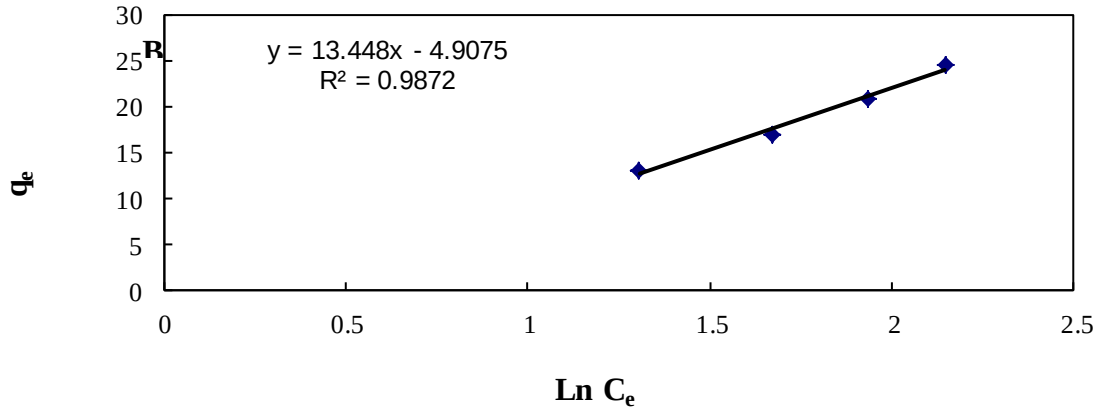


**Figure 3: Diagram of dexamethasone adsorption based on the Temkin adsorption model**

**Table 2: Calculating parameters of adsorption isotherms of Langmuir, Fruundlich and Temkin for dexamethasone adsorption on the single-walled carbon nanotubes**

| Frundlich | Langmuir | Temkin |
|---|---|---|
| $R^2$= 0.9999 | $R^2$= 0.9099 | $R^2$= 0.9856 |
| n = 1.05 | Qm(mg/g) =588.24 | B = 25.46 |
| $K_f$(mg/g) =5.88 | $K_a$(L/mg) =0.01 | A = $e^{-0.49}$ |
| ------- | $R_L$=3.2 | b= 100.59 |

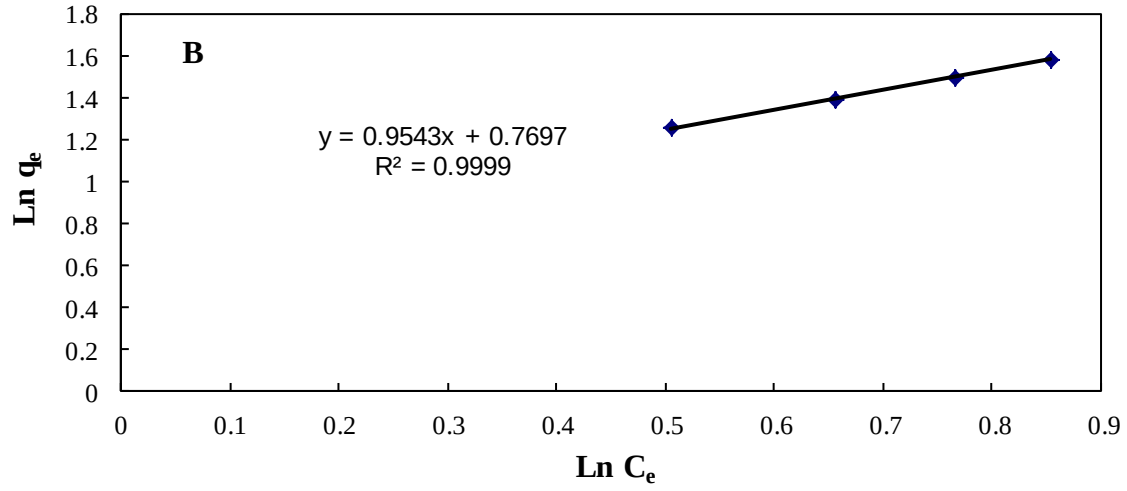


**Figure 4: Diagram of dexamethasone adsorption based on Frundlich adsorption model**

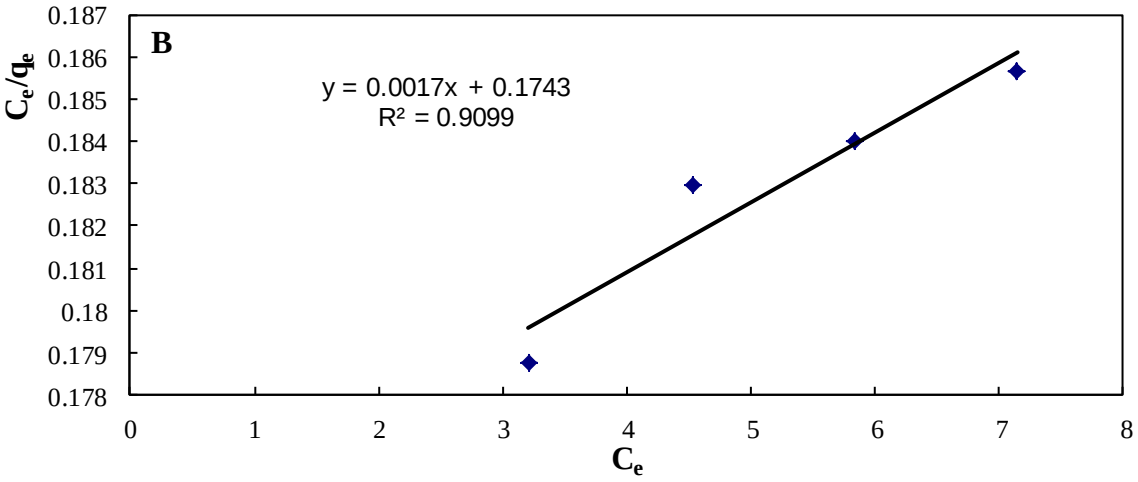


**Figure 5: Diagram of dexamethasone adsorption based on the Langmuir adsorption model**

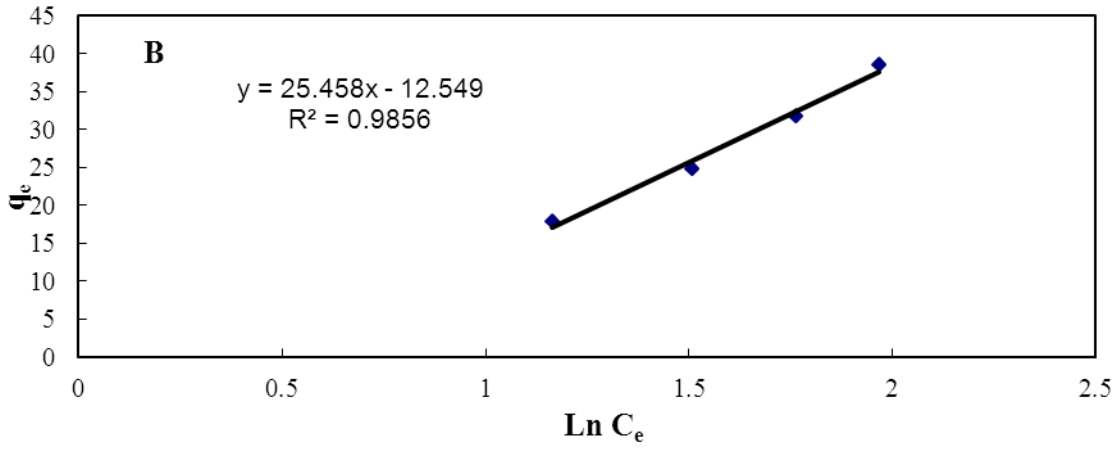


**Figure 6: Diagram of dexamethasone adsorption based on the Temkin adsorption model**

***Cimetidine***

**Table 3: Calculating parameters of adsorption isotherms of Langmuir, Frundlich and Temkin for cimetidine adsorption on multi-walled carbon nanotubes**

| Frundlich | Langmuir | Temkin |
|---|---|---|
| R2= 0.9895 | R2= 0.8288 | R2= 0.9837 |
| n = 0.73 | Qm(mg/g) =6.9 | B = 49.91 |
| Kf(mg/g) =5.8 | Ka(L/mg) =0.001 | $A = e^{-0.58}$ |
| ------- | RL=0.97 | b=51.3 |

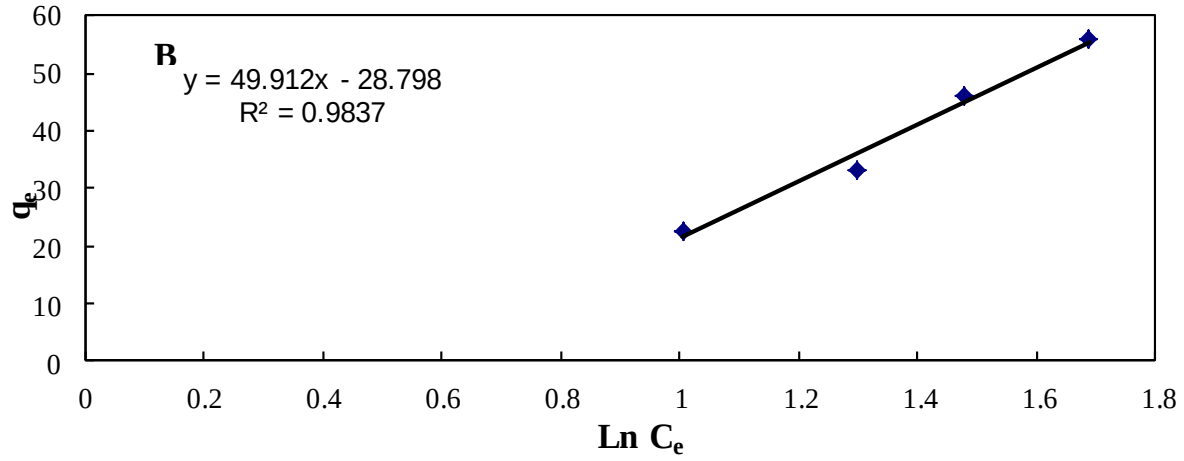


**Figure 7: Diagram of cimetidine adsorption based on the Temkin adsorption model**

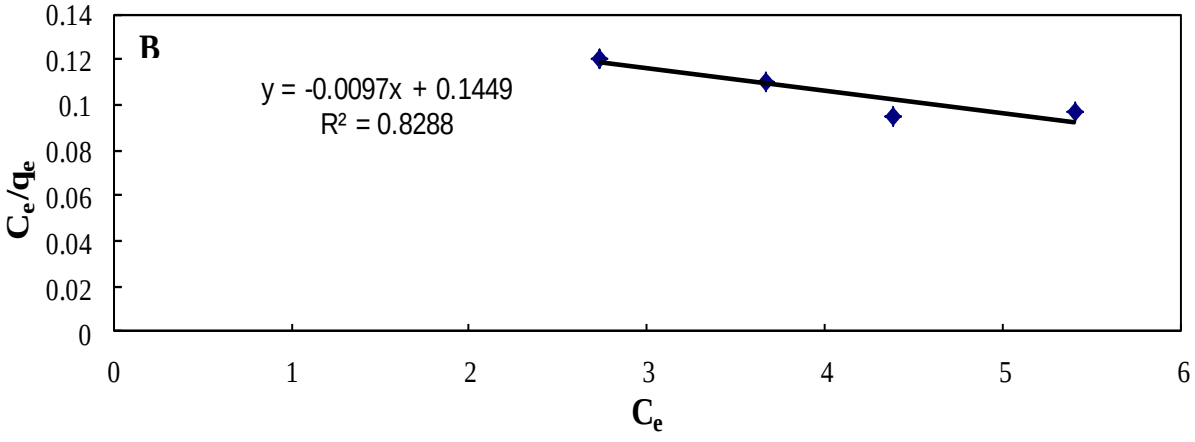


**Figure 8: Diagram of cimetidine adsorption based on the Langmuir adsorption model**

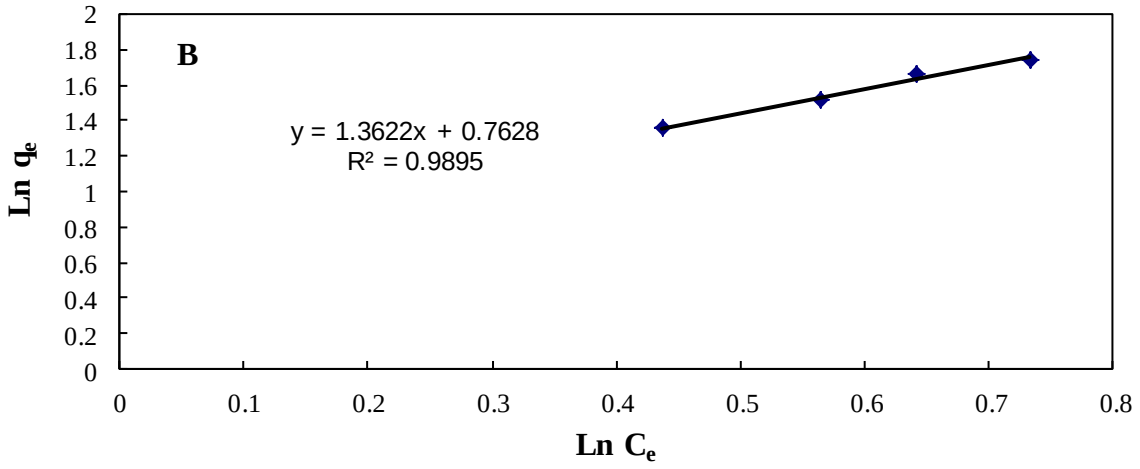


**Figure 9: Diagram of cimetidine adsorption based on the Frundlich adsorption model**

**Table 4: Calculating the parameters of adsorption isotherms of Langmuir, Frundlich and Temkin for cimetidine absorption on single-walled carbon nanotubes**

| Frundlich | Langmuir | Temkin |
|---|---|---|
| R2= 0.9981 | R2= 0.9819 | R2= 0.971 |
| n = 0.41 | Qm(mg/g) =5.78 | B = 107.39 |
| Kf(mg/g) =3 | Ka(L/mg) =0.006 | A = $e^{0.67}$ |
| ------- | RL=0.84 | b=23.84 |

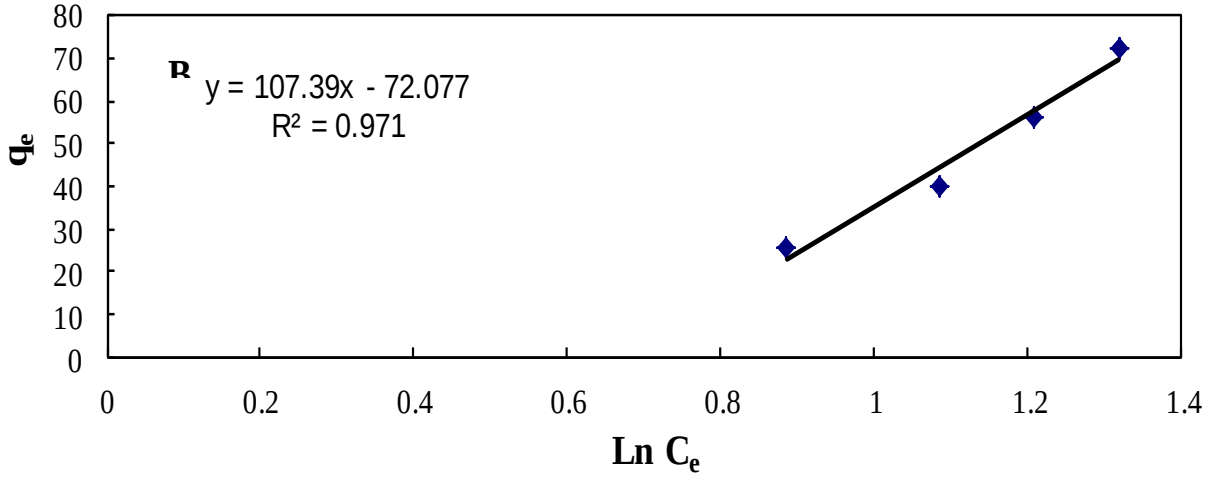


**Figure 10: Cimetidine adsorption based on the Temkin adsorption model**

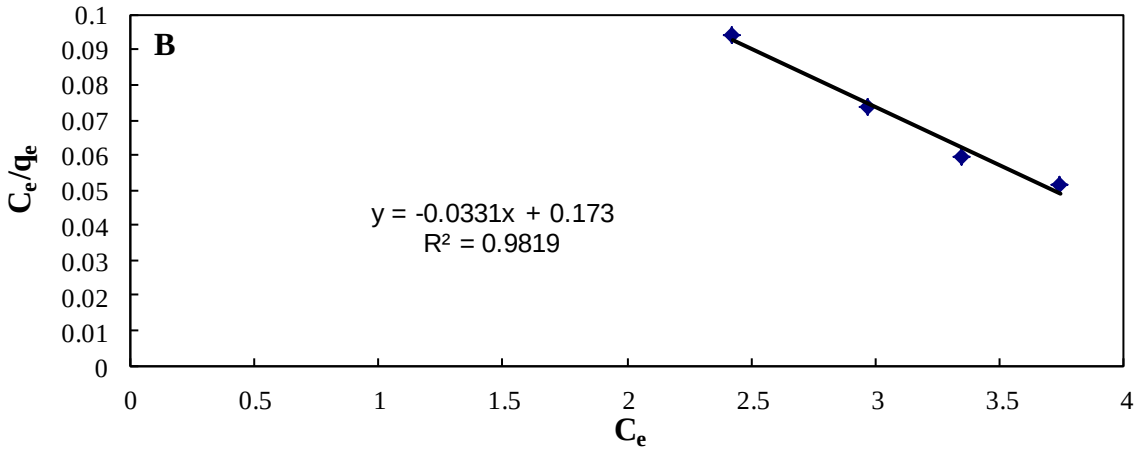


**Figure 11: cimetidine adsorption based on the Langmuir adsorption model**

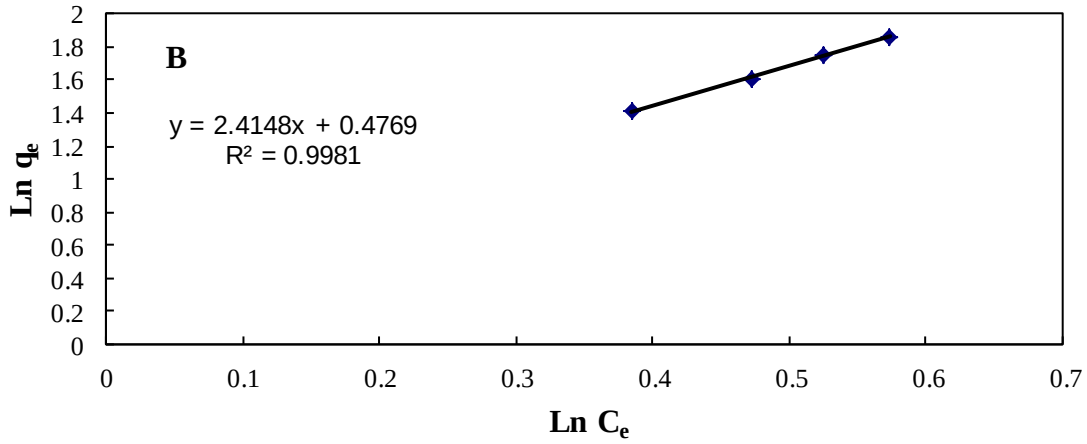


**Figure 12: cimetidine adsorption based on the Frundlich adsorption model**

***Conclusion***

According to tests carried out and on the basis of calculations made, dexamethasone and cimetidine drugs in the presence of multi-walled and single-walled carbon nanotubes will follow the Frundlich adsorption model. According to the results, the efficiency of absorption of dexamethasone and cimetidine drugs by single-walled carbon nanotube in the same conditions is more than multi-walled carbon nanotube.

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