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Isotherms and Thermodynamic Parameters of Metoprolol Drug Adsorption on the Prepared Mesoporous Silica

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Abstract

In this study, mesoporous silica (MPS) is made using the sol-gel method from a cheap source (Na2SiO3) using the surfactant hydroxycetyl hydroxyethyl dimonium chloride as a template. The task is the adsorption-based removal of the medication metoprolol (MP) at concentrations between 10 and 50 ppm. Variables such as: contact time, dose of adsorbent, starting concentration of adsorbate, and adsorption temperature were studied which show the equilibrium time and adsorbent dose are 40 min and 0.05 g respectively. The Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich isotherm models were fitted to the data obtained from the experiments. Comparing the outcomes showed that, of the four investigated isotherm models, the Freundlich equation model could accurately predict these data. Based on adsorption isotherm analysis, as the temperature was raised, it was discovered that the amount of adsorption rose and that the adsorption was advantageous and may be a physical process. In addition, the study involved estimation of ΔH°, ΔS°, and ΔG° as thermodynamic parameters. ΔG° values were discovered to be between -20.24 and -26.22 kJ/mol and reduced when temperature rose, indicating that adsorption may be become more spontaneous at higher temperatures. The value of ΔH° was 38.10 kJ/mol indicate adsorption process was physical in character. ΔS° for this process had a value of 199.14 J/mol K which suggested the increased degree of flexibility of the adsorbed MP. The sign of ΔG° and ΔH° were suggested spontaneous and endothermic of the process.

Keywords: Adsorption, Freundlich model, Isotherm, Mesoporous silica, Metoprolol.

Introduction

In recent years, the use of drugs increased, and abuse has become more common. Because drugs or their metabolites are relatively stable in the environment and difficult to control using conventional methods, these conditions cause drugs or their metabolites to persist in the environment[1]. The report of World Health Organization (WHO) at 2012[2] agree the pharmaceuticals concentrations in the treated water are typically lower than 0.05 µg L^{-1} and less than 0.1 µg L^{-1} in partially treated water. The harmful impact of drugs on the environment has been raised because their widespread exposure to medicines .From different water sources, residues reenter people's and animals' bodies and have negative effects such drug resistance and disruptions to metabolism[3]. As a result, it is urgent to remove medicines from waste water resources in order to protect the ecosystem .

Although many other methods such as, photodegradation[4], microfiltration–reverse osmosis[5], Microbial degradation[6], have been used to remove contaminants, adsorption appears promise for a number of reasons .Adsorption, for instance, outperforms other water treatment methods due to its

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lower initial cost, higher efficiency, straightforward design, and lower maintenance requirements . Adsorption also has little effect on the production of dangerous substances[4] .
One of the main contaminants in wastewater treatment plants' effluent is metoprolol .Since over 50% of metoprolol is discharged into surface waters, its low biodegradability was a selection criterion[7,8].

The purpose of this work was to clarify the function of adsorption of metoprolol onto mesoporous silica substrates .To comprehend drug adsorption onto the silica surface, adsorption isotherms were created .To further support the adsorption process' exothermic or endothermic behavior, the thermodynamic parameters were further examined.

Materials and Methods

Materials

Adsorbate: The adsorbate solutions were made using metoprolol tartrate (Sigma-Aldrich, USA), IUPAC calls this compound bis (1-[4-(2-methoxyethyl) phenoxy [3](propan-2-yl)amino[Propan-2-ol, chemical formula $(C_{15}H_{25}NO_3)_2C_4H_6O_6$),Molar mass: 685.81 g/mol; water solubility: 50 g/L; maximum absorption at wavelength 274 nm. Fig.1 depicts the chemical structure of metoprolol tartrate.

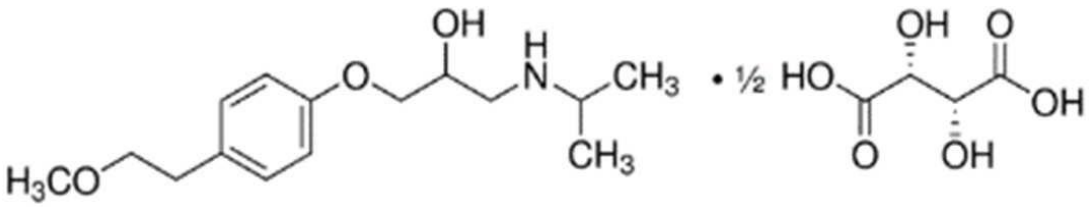

Figure 1. Chemical structure of metoprolol tartrate

Adsorbent: Using sodium silicate (14% NaOH, 27% SiO_2 w/w) as a source of silica and hydroxycetyl hydroxy ethyl dimonium chloride (dehyquart) surfactant as a template, both of which were obtained from the state company of vegetable oils in Iraq, the process for making mesoporous silica as an adsorbent is similar to the one we reported earlier[9].

The produced silica materials results of surface area and pore characteristics, as determined by adsorption-desorption analysis with a Quantachrome Instruments' Autosorb-1 (Boynton Beach, Florida, USA), are as follows: BJH pore volume and pore diameter are 0.923 cm^3g^{-1} and 1.12 nm, respectively, whereas BET surface area is 1828.9 m^2g^{-1}.

Adsorption Experiments

Experiments for metoprolol adsorption were carried out in batch mode. These tests primarily sought to determine adsorbent dose, temperature, and the equilibrium time of adsorption.

A specific amount of mesoporous silica sample was put into conical flask and 100 mL of MP medication was added, and the mixture was agitated on thermostatic shaker. After that, one milliliter of the solution was pipetted and centrifuged at 1000 rpm to separate the two components for 10 minutes. The UV-Vis technique was used to determine residual MP concentration. Effect of MP different initial concentrations (10-50 ppm) and different temperatures (293-313 K) on adsorption process was examined.

The Eq. (1) and (2) were applied to estimate the amount adsorbed (q_e) mg/g and the percentage of removal (R%) for MP[10]:

$$R\% = \left[\frac{(C_o - C_e)}{C_o}\right] \times 100 \qquad 1$$

$$q_e = \frac{(C_o - C_e) \times V}{m} \qquad 2$$

where C_o (mg/L) equal to the drug initial concentration; C_e (mg/L) equal to the drug concentration after reaching equilibrium; V(L) is the volume of the solution used in the adsorption experiment; m(g) equal to mass of mesoporous silica as adsorbent.

Adsorption Models

According to Table 1, the Freundlich, Langmuir, Temkin, and Dubinin-Radushkevich adsorption

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equations were applied to fit the experimental data from adsorption process. Also, by selecting specific slope and intercept values from the plots, constants needed for an exact comparison between them were found.

Table 1. The adsorption models used in this work

Name	Equation (Linear form)	Plot	Slope	Intercept
Langmuir	$\boldsymbol{Ce/qe} = \mathbf{1}/\boldsymbol{q_m}K_L + \boldsymbol{Ce/q_m}$	$\boldsymbol{Ce/qe}$ vs. C_e	$\mathbf{1}/\boldsymbol{q_m}$	$\mathbf{1}/\boldsymbol{q_m}K_L$
Freundlich	$\log q_e = \log K_f + \mathbf{1}/\boldsymbol{n}\log C_e$	logqe vs. log C_e	$\mathbf{1}/\boldsymbol{n}$	log K_f
Temkin	$q_e = B \ln K_t + B \ln C_e$	q_e vs. $\ln C_e$	B	B ln K_t
Dubinin- Radushkevich	$\ln q_e = \ln q_m - \beta\epsilon^2$	$\ln q_e$ vs. ϵ^2	β	$\ln q_m$

Where K_F (Freundlich constant) stands for the adsorption capacity (L/g), K_L (Langmuir constant) refers to the affinity of the binding sites (L/mg), and q_m for maximal adsorption capacity necessary to create the monolayer. B is constant of Timken where B = RT / b and b is an equilibrium constant, β is related to mean sorption energy E (J/mol) through the equation: $E = (-2\beta)^{-0.5}$, and **ε** is the Polanyi potential described as**:** $\boldsymbol{\varepsilon} = RT \ln (1 + 1/C_e)$.

Results and discussion

Effect of adsorbent weight and contact time

Fig. 2, A displays the removal percent (R%) and amount adsorbed (qe) of 15 ppm MP medication against the weight of MPS adsorbent at 293 K. From this graph, it can be shown that the MP medication clearance and amount adsorbed rise as the weight of MPS increases up to 0.05 g in aqueous solution. This is explained by a rise in the MPS's surface area, which raises the number of binding sites. Higher dosages result in a very quick adsorption onto the adsorbent surface, which improves drug absorption[11,12].

Fig. 2, B, which depicts the rapid increase in the amount adsorbed as contact time increase up to 40 minutes in which the high value is shown, provides an illustration of the impact of contact time on adsorption. The availability of adsorption sites of the adsorbents got diminished, leading the amount adsorbed to be constant[13], so all adsorption studies were conducted at this equilibrium time (40 min) and at 0.05 g adsorbent dose.

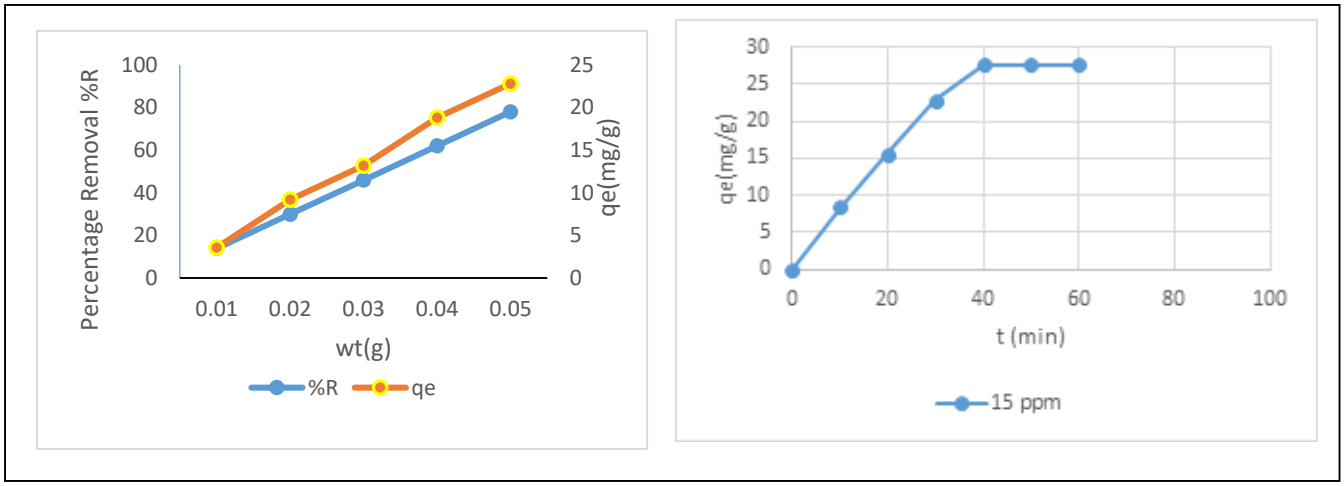

Figure 2. Effect of adsorbent dose and equilibrium time on MP adsorption.

Adsorption isotherm

Adsorption isotherms of MP on the MPS surface using four temperatures ranged from 293 – 333 K and initial concentrations ranged from 10 -50 ppm are presented in Fig. 3.

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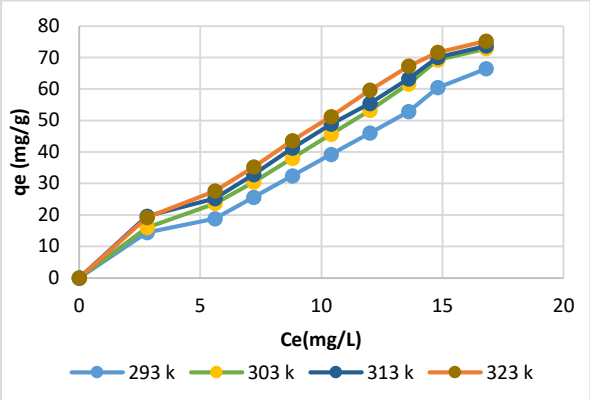

Figure 3. Adsorption isotherms of metoprolol /mesoporous silica system.

Fig.3 demonstrates that as temperature rises, MP adsorption increases, indicating that the operation is endothermic. This can be taken to mean that when temperature rises, collisions occur more frequently. High temperatures may also increase activation energy or porous dimension[14]. With increasing initial concentration of MP drug from 10 to 50 mg/L, the q_e of drug molecules increases from 14.4to 66.4 after 40 min of equilibrium adsorption time. On the other hand, Fig. 3 shows adsorption isotherms at low MP concentrations, yielding an S-type (or Type V) isotherm[15]. This indicates that the direct interaction between the adsorbent surface and metoprolol molecules is low, and only after obtaining some coverage, adsorption increase. A similar observation was made for several pharmaceuticals in previous studies[16 -18].

Finding a suitable model to be employed requires analyzing the experimental data and fitting it in various isotherm equations[19]. These isotherm equations are Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich. The parameters obtained in the fitting, along with a correlation coefficient (R^2), are present in Table 2 while typical linear plots of the four models are shown in fig.4.

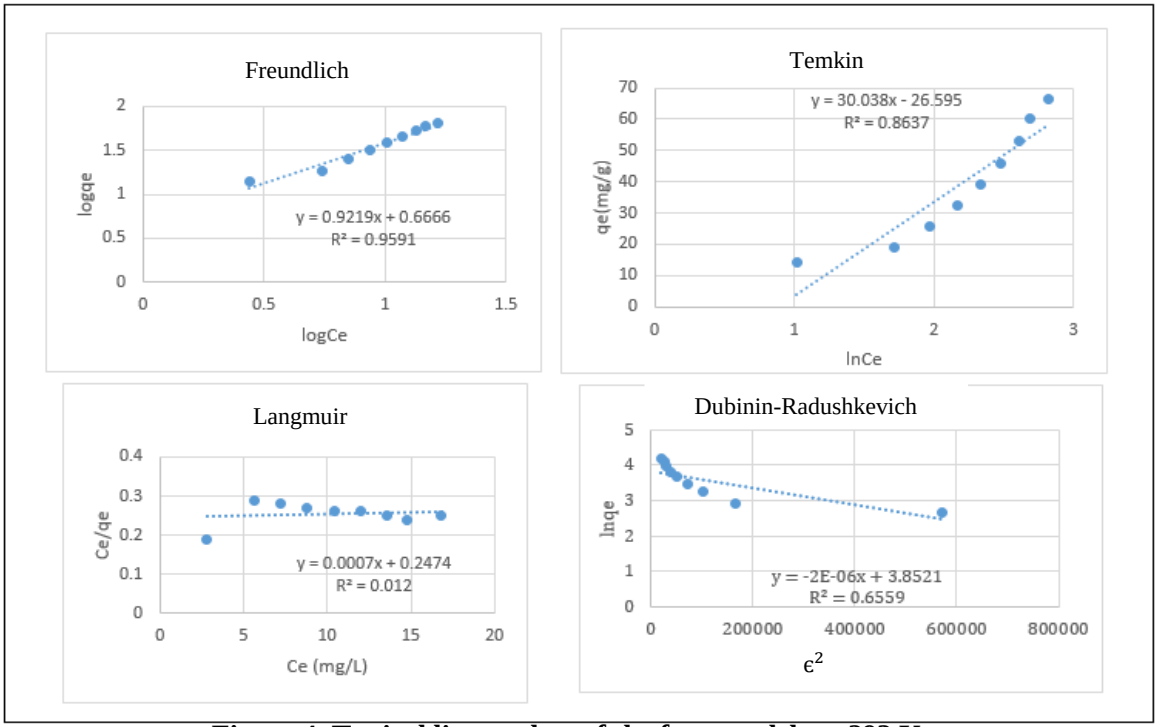

Figure 4. Typical linear plots of the four models at 293 K.

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Table 2. The four models' parameters for the adsorption process.

Isotherm	Parameters	Temperature			
		293K	303K	313K	323K
Langmuir	q_m(mg/g)	1428	321	149	94.33
	K_L(L/mg)	0.0028	0.026	0.092	0.38
	R_L	0.959	0.719	0.42	0.149
	R^2	0.0120	0.6825	0.9941	0.9742
Freundlich	1/n	0.921	0.848	0.731	0.434
	K_f (L .g^{-1})	1.94	2.55	3.02	4.1
	R^2	0.959	0.985	0.974	0.975
Temkin	B(L/mg)	30.038	32.123	27.96	18.111
	K_T(J/mol)	0.412	0.664	1.066	4.673
	R^2	0.8637	0.9306	0.976	0.9251
Dubinin- Radushkevich	β(mol^2 J^{-2})	-2×10^{-6}	-1×10^{-6}	-1×10^{-6}	1×10^{-7}
	qm(mg\g)	47.091	58.061	61.135	55.135
	E(kJ/mol)	0.500	0.707	0.707	0.022
	R^2	0.6559	0.8028	0.8679	0.6707

Table2. results show that the highest adsorption capacity (q_{max}) according to Langmuir model ranged from 94.33 to 1428 mg/g and declined as the temperature range under study was expanded. The results also show a low value of R^2 (0.0120 - 0.994). These findings show that the experimental data could not be explained by the Langmuir equation, indicating that this model is unsuitable for analyzing the experimental data of MP adsorption on MPS.

With the range of temperatures investigated, KF constant associated to adsorption capacity ranged from 1.94 to 4.10 L/g. The fact that KF's value grew as the temperature rose suggests endothermic nature of the adsorption process. If n equals one, adsorption is linear; if n less than one, the process is a chemisorption type; and if n exceeds one, the process is physisorption type[20]. The n value shows the degree of nonlinearity between solution concentration and adsorption. According to Table 2, the range for 1/n was between 0.434 and 0.921 at 293 and 323 K. To put it another way, the n value is between 1.08 and 2.30 for all tested temperatures, which indicates that MP was physically and favorably adsorbed onto silica[21, 22].The equilibrium data had an R^2 value of 0.959 to 0.985, which fit the Freundlich expression.

The Temkin isotherm's highest binding energy was connected to an equilibrium binding constant (K_T) that ranged from 0.412 to 4.673 J/mol. The relationship between K_T and temperature increased, demonstrating that the adsorption process's physical connection between MP and silica surface and grew stronger as temperature rose.

E, the adsorption energy determined by Dubinin- Radushkevich models, ranged from 0.0223 to 0.707 kJ/mol which are less than 8 kJ/mol. These outcomes further validate that the process is physical adsorption procedure[23]. The equilibrium data had an R^2value of 0.8637 -0.976 for the Temkin expression and 0.6559 -0.8679 for the Dubinin- Radushkevich expression.

According to these results, the maximum R^2 values are in the range 0.959 - 0.985 for the Freundlich model. This confirm the Freundlich model was the optimum model for the adsorption of MP drug onto mesoporous silica. The produced mesoporous silica's surface is likely heterogeneous, with interactions between MP molecules on the surface, according to the Freundlich isotherm's excellent fit to the experimental data[24].

Thermodynamic study

To assess the viability and the adsorption process nature, thermodynamic parameters (ΔG°), (ΔH°), and (ΔS°) were determined[25]. The following Eq. (3) and (4)[26], are used to estimate them and the expression Keq = qe / Ce was used to calculate Keq, the equilibrium constant.

$$\Delta G^\circ = -RTlnK_{eq} \qquad 3$$

$$lnK_{eq} = \frac{-\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R} \qquad 4$$

As illustrated in Fig.5, the linear relationship between the ln Keq plot against 1/T of Eq.4 and the

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values of ΔH° and ΔS° can be inferred from the slope and intercept. Table 3. contains the calculated thermodynamic parameters.

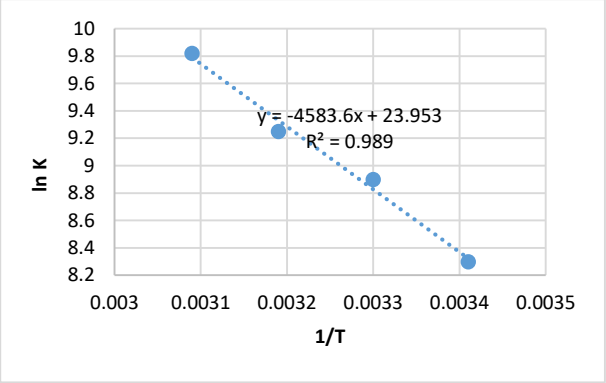

Figure 5. The vant Hoff plot of the adsorption of MP on MPS process.

Table 3. The thermodynamic function of the adsorption of MP on MPS.

Temperature(K)	ΔH˚ kJ/mol	ΔS˚J/mol K	Δ G˚ kJ/mol
293	38.10	199.14	- 20.24
303			-22.23
313			-24.23
323			-26.22

As shown from Table 3. The value of ΔH° was 38.10 kJ/mol indicate adsorption of MP drug on MPS surface was physical in character and involved weak attraction between them. ΔH° value of less than 40 kJ/mol indicates the physical adsorption of the adsorbate molecules and the adsorbent surface[27]. Additionally, the fact that ΔH° is positive shows the endothermic nature of adsorption.

ΔG° values were discovered to be between -20.24 and -26.22 kJ/mol and reduced when temperature rose, indicating that adsorption may be become more spontaneous at higher temperatures. Higher negative values represent an adsorption process that is more energy-beneficial, and the ΔG° measures the spontaneity of the adsorption process. The study's negative ΔG° values at all temperatures under investigation attest to the adsorbent's viability and the spontaneity of adsorption [28, 29].

ΔS° for this process had a value of 199.14 J/mol K. The increased degree of flexibility of the adsorbed MP is suggested by the positive value of ΔS°. Based on this finding, it was shown that MP adsorption improves the randomness of the overall system while water molecules surrounding it were released during adsorption.

Conclusion

In a batch experimental setting, the MP drug adsorption from an aqueous solution onto MPS was investigated. Langmuir, Freundlich, Temkin and Dubinin-Radushkevich models of adsorption isotherm were employed to examine the experimental data of MP onto MPS. It was discovered that adsorption was advantageous, that its capacity increased with temperature, and that it was a physical process. When the results of the four different adsorption models were compared, it became clear that the Freundlich model had the highest accuracy in its ability to explain the MP adsorption equilibrium data, indicating a heterogeneous surface with interactions between the MP and MPS. The adsorption thermodynamics results indicate that (1) the adsorption of MP on MPS was;(1) physisorption, and tended to be endothermic, (2) spontaneous, and became more spontaneous at higher temperatures, and (3) increased randomness at the solid/liquid interface.

Author's Declaration

The authors would like to declare that there is no conflict of interests, hereby declare that this submission is entirely our own work, in our own words, and that all sources used in researching it are fully acknowledged and all quotations properly identified. It has not been submitted, in whole or in part, by me or another person, for the purpose of obtaining any other credit / grade. We understand the ethical implications of our research, and this work meets the requirements of the Faculty of Science, Sciences Research Ethics Committee.

Author's Contribution

S. H. K. suggested and planned the research idea.
M. A. S. designed and carried out the experiments.
All authors contributed in the analysis and discussing of the results and writing the manuscript.

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الايزوثيرمات والدوال الدينميكية الحرارية لامتزاز دواء الميتوبرولول على السليكا متوسطة المسام المحضرة

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قسم الكيمياء، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق.

الخلاصة

في هذه الدراسة ، تم تصنيع السيليكا متوسطة المسام ((MPS) باستخدام طريقة سول-جل من مصدر رخيص (Na_2SiO_3)باستخدام هيدروكسي ستيل هيدروكسي إيثيل دايمونيوم كلوريد كقالب. وتتمثل المهمة في الإزالة القائمة على الامتزاز لعقار ميتوبرولول (MP) بتراكيز تتراوح بين 10 و50 جزء في المليون. تمت دراسة المتغيرات مثل: وقت التلامس، كمية المادة المازة، التراكيز الابتدائية للمادة الممتزة، ودرجة حرارة الامتزاز، ودلت النتائج ان زمن الاتزان وكمية المادة المازة هما 40 دقيقة و 0,05 غرام على التوالي. تم تطبيق ايزوثرمات Temkin, Freundlich , Langmuir وDubinin-Radushkevich على البيانات التي تم الحصول عليها من التجارب و قد أظهرت مقارنة النتائج أنه ، من بين نماذج الايزوثرمات الأربعة التي تم فحصها ، يمكن لنموذج معادلة Freundlich التنبؤ بهذه البيانات بدقة. وبالاعتماد على تحليل ايزوثرم الامتزاز تبين انه مع ارتفاع درجة الحرارة أن كمية الامتزاز ارتفعت وأن الامتزاز كان مفيدًا ومن النوع الفيزيائي. بالإضافة إلى ذلك، تضمنت الدراسة تقدير $\Delta G°$,$\Delta S°$, $\Delta H°$, كعوامل ديناميكية حرارية. ووجد ان قيمة $\Delta G°$ كانت بين -20,24 و -26,22 كيلوجول لكل مول وتقل مع ارتفاع درجة الحرارة مما يدل على ان الامتزاز يصبح اكثر تلقائية بدرجات الحرارة العالية. كانت قيمة $\Delta H°$ هي 38.10 كيلوجول لكل مول والتي دلت بان عملية الامتزاز من نوع الامتزاز الفيزيائي. اما قيمة $\Delta S°$ فكانت 199.14 جول لكل مول والتي تدل عل زيادة درجات الحرية للمادة الممتزة MP. ودلت اشارة $\Delta G°$ و $\Delta H°$ بان العملية تلقائية وماصة للحرارة.

الكلمات المفتاحية: امتزاز، ايزوثرم، ميزوبورس سليكا، ميتوبرولول، نموذج فرندلش.