Computational study on the corrosion inhibition of nano materials of Zn, Al, Fe and Cu by clindamycin

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Abstract

Clindamycin an antibacterial drug was assessed for its potential as a corrosion inhibitor for Al, Zn, Cu and Fe metals, the optimized structures were used for calculating their quantum chemical properties and the values of Log P (0.79) and free Gibbs energy (-0.00258) of the inhibitor confirms the spontaneous nature of clindamycin, other QSPR parameters such as hardness, softness, EA, IP and total energy (E) were also calculated and correlated with the binding energy of clindamycin with their respective surfaces. The inhibitor was used for a molecular dynamic simulation study using Material Studio 7 software and the binding energies of clindamycin on the selected metal surfaces were determined via quenching process and Monte Carlo algorithm. The energy of the metals was found to be significantly correlated with the binding energy and hence it was used in the development of a QSPR model (Binding Energy = -70.833*E (kJ/mol) - 106.348) via GFA method for predicting the binding energy of clindamycin with any metal surface, the model was found to be significant and the R2 and CVR2 were found to be 0.976 and 0.765 respectively.

Keywords: Clindamycin; Binding energy; Corrosion inhibitor; QSPR; Adsorption; Drug.

Introduction

Corrosion in various media is a significant problem that normally causes things made of compressed composition of metals to flop in the factory and industrial spaces, structures such as steel rebar corrosion in solid constructions. Corrosion resistance is also a property of a metal that gives it the ability to withstand attacks from chemical, or electrochemical conditions, but these metals no matter how tough can only withstand corrosion for a while.

Over the past decade, several corrosion experimental methods have been industrialized for the analysis of corrosion difficulties, for the forecast of care requirement, and for the identification of the most effective inhibitor and optimum inhibitor dosages [1]. Organic compounds have been
described in the books as some of the most effective corrosion inhibitors, due to the fact that most of them have lone pair electrons found in heteroatoms present as a motif of their structure (P, S, N, and O) [2,3]. However, the use of most of these substances has been hindered, due to a number of uncomfortable side effects they trigger inside the environment [4]. Thus, this development with the novel corrosion inhibitors regarding its low toxicity has been regarded as a much more important casing point [5,6].

Because they are basically synthesized from natural occurring phytochemicals [7,8], as well as their environmentally friendly properties [9] and also minimal adverse influences around the aquatic surroundings [10], drugs (chemical medicines) seem to be suitable candidates to replace standard poisonous corrosion inhibitors.

On expenses of aforementioned structural differences, corrosion inhibition potentials of most studied drugs have attracted a good number of interest in recent years. This paper provides a theoretical insight into the use of antibacterial drug Clindamycin as a potential corrosion inhibitor, recent developments that have been reported in the literature shows that it is a fairly good inhibitor for corrosion of Zinc in a minimum concentration of sulphuric acid [8]. The main aim is to identify the binding affinity of this drug to a group of metals and compare for them for its optimum use as a corrosion inhibitor.

Corrosion scientists are attempting to integrate environmental considerations directly into corrosion inhibitor selection processes, in order to respond to an increased awareness of the need to protect the environment [11]. Some of the drugs reported to have shown an impressive potential as corrosion inhibitors includes Penicillin G [12], penicillin V[13], Ampicillin [11], cloxacillin [5], cefixime [14] , Norfloxacin [15], quinolone, quinaldine and quinaldic acid [1] . Intense research by several groups has produced some models, but none of these have enough experimental backup to be identified as the true inhibition mechanism [16,17]. Further research, both theoretical and experimental, remains vital.

**Materials and Methods**

**Computational Detail**

The present calculations were achieved by means of Spartan 14 V 1.1.4 (Wavefunction program package [18].

![Figure 1: The molecular structures of the investigated inhibitor (Clindamycin)](image)

Geometry optimization of clindamycin was carried-out via Density Functional Theory by employing Becke’s three parameter ex-change functional (B3LYP) [19,20,21], and embraces DFT electron exchange functionals coupled with the
Electronegativity, softness, and hardness are important quantities in theorizing the reactivity of chemicals. When clindamycin is brought to the metal surface it is expected that electrons will flow from lesser value $\chi$ (clindamycin) to higher $\chi$ (Metal), until the chemical potentials become equal. Hence the total number of transferred electrons ($\Delta N$) was calculated using equation 6

$$\Delta N = (\chi_{\text{Metal}} - \chi_{\text{inh}})/2(\eta_{\text{Metal}} + \eta_{\text{inh}}) \quad \text{(6)}$$

Where $\eta_{\text{Metal}}$ and $\eta_{\text{inh}}$ in equation (6) represents the total electronegativity of iron and clindamycin respectively, while $\chi_{\text{Metal}}$ and $\chi_{\text{inh}}$ represent the absolute hardness of the metal and clindamycin respectively [22].

The change in electronegativity initiates the electron transfer, and the addition of the hardness parameter acts as a struggle or opposition to the electron flow. The total electrophilicity index was developed by Parr [13,17,18] and is given as

$$\omega = \mu^2/2\eta \quad \text{(7)}$$

According to equation 7, this index parameter measures the tendency of chemical species to accept electrons. A good responsive nucleophile is considered by the insignificant value of $\chi$ and $\omega$ (equation 7), while for an effective electrophile a significant value of $\omega$ and $\chi$ is noticed.

This paper aims to extend these inquiries in order to confer the link between quantum chemical calculations and Binding energy of clindamycin on various considered metals (Fe, Al, ZnO, and Cu) by defining the quantum chemical descriptors responsible for this inhibition efficacy of clindamycin, this parameters includes the energies of the lowest unoccupied molecular orbital (ELUMO) and highest occupied molecular orbital (EHOMO), the energy difference (DE) between EHOMO and ELUMO, dipole moment ($l$), softness ($\sigma$),
electron affinity (A), global hardness (η), ionization potential (I), the portion of electrons transferred (ΔN), electronegativity (v), and the total energy (TE)

**Result and Discussion**

Wang et al. [23], specified that the frontier orbital (highest occupied molecular orbital-HOMO and lowest unoccupied molecular orbital-LUMO) of a chemical species play a significant part in defining its reactivity.

![Figure 2](image)

**Figure 2:** Electronic properties of Clindamycin: (a) optimized structure, (b) HOMO orbital, (c) LUMO orbital and (d) total electron density (atom legend: light gray H, dark gray C, red O, purple Cl, yellow S and light green N). The isosurfaces (larger lobes) depict the electron density difference; the darker regions show electron accumulation, whereas the lighter regions show electron loss.

As EHOMO is frequently linked with the electron giving ability of a molecule, high value of EHOMO are expected to show the tendency of the molecule to donate electrons to appropriate acceptor molecules with lower energy molecular orbital [19,24]. Increasing values of EHOMO facilitate adsorption and therefore enhance the inhibition efficiency, by influencing the transport process through the adsorbed layer. Table 1 shows the quantitative structural properties related parameter computed using a DFT method, the area of molecule was given as 424.26 Armstrong, while the free Gibbs energy is given as -0.00258 au. The result is evident on the reported experiment analysis on the spontaneity and surface area of the molecule for efficient adsorption of the molecule on Zn surface and truly in this context metal surface.
Table 1: Quantitative Structural Property Related parameters for Clindamycin calculated using B3LYP/6-311 ++ G(d,p).

The value of hydrophobicity (Log P) which defines the lipophilicity or hydrophobicity of a compound is high (0.79) signifying the ability of the drug to protect the surface of the metal from an attack of corrosive agents directly on the metal surface. Other quantum chemical parameters like ELUMO presented in Table 2, indicates the ability of the molecule to accept electrons, hence the binding ability of the inhibitor to a metal surface, and influenced by increasing of the HOMO and decreasing of the LUMO energy values of Clindamycin. Frontier molecular orbital diagrams of Clindamycin are presented in Figure 2. According to the frontier molecular orbital theory (FMO) of chemical reactivity, the transition of electron is due to interaction between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of reacting species [25,26].The higher values of EHOMO of clindamycin will donate electrons to orbital of iron (Fe), followed by copper (Cu) and finally aluminium (Al), zinc is found to have a much higher EHOMO and lower ELUMO than that of the inhibitor, thereby retarding the possibility of clindamycin adsorbing on zinc surface and decreasing the overall corrosion inhibition potential of clindamycin in zinc environment, hence the higher the corrosion inhibition efficiency through better adsorption.

<table>
<thead>
<tr>
<th>Area (Å²)</th>
<th>Log P</th>
<th>Polarizability</th>
<th>HBD</th>
<th>HBA</th>
<th>Ovality</th>
<th>S° (kJ/mol)</th>
<th>H°(kJ/mol)</th>
<th>G°(kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>424.26</td>
<td>0.79</td>
<td>72.66</td>
<td>4</td>
<td>8</td>
<td>1.58</td>
<td>0.679</td>
<td>195.68</td>
<td>-6.77</td>
</tr>
</tbody>
</table>

Clindamycin | Zinc (Zn) | Copper (Cu) | Iron (Fe) | Aluminium (Al) |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>E (kJ/mol)</td>
<td>-1104.16</td>
<td>130.42</td>
<td>337.65</td>
<td>786.06</td>
</tr>
<tr>
<td>E HOMO (kJ/mol)</td>
<td>-861.52</td>
<td>-900.54</td>
<td>-806.78</td>
<td>-742.73</td>
</tr>
<tr>
<td>E LUMO (kJ/mol)</td>
<td>21.21</td>
<td>-156.76</td>
<td>12191.22</td>
<td>279.52</td>
</tr>
<tr>
<td>IP (kJ/mol)</td>
<td>861.52</td>
<td>900.54</td>
<td>806.78</td>
<td>742.73</td>
</tr>
<tr>
<td>EA (kJ/mol)</td>
<td>-21.21</td>
<td>156.76</td>
<td>-12191.22</td>
<td>-279.52</td>
</tr>
<tr>
<td>Hardness (kJ/mol)</td>
<td>441.365</td>
<td>371.89</td>
<td>6499</td>
<td>511.125</td>
</tr>
<tr>
<td>Softness (kJ/mol)</td>
<td>0.002265</td>
<td>0.002689</td>
<td>0.000154</td>
<td>0.001956</td>
</tr>
<tr>
<td>Global electrophilicity index</td>
<td>-7871208.2</td>
<td>-63564008.2</td>
<td>-396759578</td>
<td>-77098303.9</td>
</tr>
</tbody>
</table>
Absolute softness and hardness are significant properties to measure in understanding the molecular stability and reactivity of clindamycin with the surface of the metal. It is important to note that the absolute chemical hardness is fundamentally responsible for the resistance given towards the deformation or polarization of the electron cloud of the atoms, molecules and ions under small trepidation of chemical reaction agrees with the result of the ionization potential (IP) and electron affinity of the species presented in Table 2 (EA). Aluminium is found to have the smallest hardness (331.87 kJ/mol) and highest softness value (0.0030 kJ/mol) making it the least reactive surface with an exception of Zinc whose value deviates from those of the other metals because of its stability corresponding with the completely filled d-orbital it outermost shell. The ΔN values were presented in Table 2, this represents the total number of electronic charges that will be conveyed between the surface and the adsorbed species. The larger value of -0.145 for Fe signifies the maximum transfer of electron and hence greater inhibition efficiency, while the least transferred electron was noticed in Cu (0.579) hence signifying the possibility of finding the least corrosion inhibition property of clindamycin.

The correlation analysis of the binding energy of the metal to the inhibitor (clindamycin) presented in Table 3. It showed that their binding energies (Fe, Al, Zn and Cu) inversely correlated with the total energy of the metals studied; the correlation was significant at 99% confidence interval. Pearson correlation test revealed that the decrease in energy of the metals increase the binding energy of the inhibitor to the metal complex.

**Molecular dynamics simulation**

In order to model various low energy conformations and find the energy minima, molecular dynamics (MD) virtual reality of the interactions between a single molecule of interest and Fe/Al/Cu/ZnO surface was done by means of Forcite quench molecular dynamics cutting-edge Material Studio (MS) 7.0 program. Computations on the inhibitor interaction with the metal surface measured was carried out using COMPASS II forcefield and Smart algorithm in a simulation box 17Å x 12 Å x 28 Å with an intermittent limit situation, to model a functional part of the Fe/Al/Cu/ZnO slab and a vacuum layer of 20 Å height. The metal’s model was hewn beside the (110) plane with a fractional distance of 3.0 Å.
Table 3: Pearson Correlation Analysis of Quantum chemical Properties and the Binding Energy of Clindamycin with the Considered Metal Surfaces.

<table>
<thead>
<tr>
<th></th>
<th>ZnO</th>
<th>CuO</th>
<th>NiO</th>
<th>AgO</th>
</tr>
</thead>
<tbody>
<tr>
<td>ELUMO</td>
<td>0.027</td>
<td>-0.999</td>
<td>-0.228</td>
<td>1</td>
</tr>
<tr>
<td>IP</td>
<td>0.356</td>
<td>-0.277</td>
<td>-1</td>
<td>0.225</td>
</tr>
<tr>
<td>EA</td>
<td>-0.027</td>
<td>0.099</td>
<td>0.227</td>
<td>-1</td>
</tr>
<tr>
<td>Hardness</td>
<td>0.034</td>
<td>-0.105</td>
<td>-0.249</td>
<td>0.999*</td>
</tr>
<tr>
<td>Softness</td>
<td>0.218</td>
<td>-0.168</td>
<td>0.332</td>
<td>-0.944*</td>
</tr>
<tr>
<td>Global electrophilicity</td>
<td>-0.027</td>
<td>0.100</td>
<td>0.228</td>
<td>-1</td>
</tr>
<tr>
<td>ΔN</td>
<td>0.276</td>
<td>-0.327</td>
<td>-0.451</td>
<td>0.955*</td>
</tr>
<tr>
<td>Molecular Wt.</td>
<td>0.102</td>
<td>-0.038</td>
<td>-0.954</td>
<td>0.389</td>
</tr>
</tbody>
</table>

* Significant at 99% confidence interval

For cite optimized structures of Clindamycin and the metal faces were utilized to mock-up all the interactions of the molecule with the surfaces [27-29]. Figure 3-6 shows the adsorption of clindamycin on all four metals, emphasizing the epitaxial adsorption pattern of the inhibitor on the several metal surface, a specific nitrogen and also oxygen atoms were obtained in all cases to be the main point of adsorption, the end of the metal surface displays that these atoms having excess lone pair of electron positions this molecule for efficient donation of electrons to the metal surface and hence supporting the result from the calculated quantum chemical parameters such as hardness, softness, IP, EA, EHOMO and ELUMO accordingly.

![Figure 3: Representative snapshots from molecular dynamics models of Clindamycin adsorption on ZnO (110), highlighting the soft epitaxial adsorption mechanism with accommodation of the molecular backbone in characteristic epitaxial grooves on the metal surface](image_url)
**Figure 4:** Molecular dynamics model of a single Clindamycin molecule adsorbed on Fe (110): (a) side view; (b) on-top view
Figure 5: Molecular dynamics model of a single Clindamycin molecule adsorbed on Cu (110): (a) side view; (b) on-top view
Figure 6: Molecular dynamics model of a single Clindamycin molecule adsorbed on Al (110): (a) side view; (b) on-top view.
Table 4: Binding Energy of the metal-inhibitor (Clindamycin) complex

<table>
<thead>
<tr>
<th>Metal-Inhibitor complex</th>
<th>Binding Energy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al-clindamycin</td>
<td>-92.880</td>
</tr>
<tr>
<td>Cu-clindamycin</td>
<td>-100.400</td>
</tr>
<tr>
<td>Fe-clindamycin</td>
<td>-202.317</td>
</tr>
<tr>
<td>ZnO-clindamycin</td>
<td>-29.796</td>
</tr>
</tbody>
</table>

The binding energy of the inhibitor on the metals surface was calculated using the relationship in Eq. 8:

\[ E_{\text{bind}} = E_{\text{total}} - (E_{\text{Mol}} + E_{\text{Fe}}) \]  

A negative value of \( E_{\text{bind}} \) corresponds to a stable adsorption structure, whereas \( E_{\text{Mol}}, E_{\text{Fe}} \) and \( E_{\text{total}} \) correspond, respectively to the total energies of the molecule, Fe (110) slab and the adsorbed Mol-Fe (110) couple in the gas phase. The total energies were calculated by averaging the energies of the five most stable representative adsorption configurations and the binding affinity of clindamycin on Fe surface was found to be the best (-202.317Kcal/mol), while that of ZnO was found to have binding affinity (-29.796), suggesting that Fe surface would be most favourable for the use of clindamycin as a corrosion inhibitor.

Table 5: Statistical Parameters of the GFA model for Binding Energy of Clindamycin on metal Surfaces

<table>
<thead>
<tr>
<th>STATISTICAL PARAMETER</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Friedman LOF</td>
<td>404.540181</td>
</tr>
<tr>
<td>R-squared</td>
<td>0.984614</td>
</tr>
<tr>
<td>Adjusted R-squared</td>
<td>0.976921</td>
</tr>
<tr>
<td>Cross validated R-squared</td>
<td>0.765784</td>
</tr>
<tr>
<td>Significant Regression</td>
<td>Yes</td>
</tr>
<tr>
<td>Significance-of-regression F-value</td>
<td>127.990485</td>
</tr>
<tr>
<td>Critical SOR F-value (95%)</td>
<td>17.416641</td>
</tr>
<tr>
<td>Replicate points</td>
<td>0</td>
</tr>
<tr>
<td>Computed experimental error</td>
<td>0</td>
</tr>
<tr>
<td>Lack-of-fit points</td>
<td>2</td>
</tr>
<tr>
<td>Min exp. error for non-significant LOF (95%)</td>
<td>5.39568</td>
</tr>
</tbody>
</table>
The genetic function approximation (GFA) is a method developed by Rogers and Hopfinger [30] has been employed to uncover significant quantitative structure-property relationship (QSPR) models. This technique brings together Holland’s hereditary protocol (GA) [31] having Friedman’s multivariate adaptive regression splines (MARS) [32]. The GFA algorithm gives a new nonlinear way for developing actual structural models such as QSPR models. The result along with statistical analysis of the model is presented in Table 5 and 6, this also confirms that a Reasonable performance was obtained with the GFA procedure with $F = 404.54$ and $1.0$ for the limit value intended for introducing variables. The $R^2$ and $CV R^2$ (Figure 7) were 0.976 and 0.765, respectively, the advantages of GFA over other methods for modelling could be due to a particular introduction, connected with spline terms in making Quantitative Structure-Property Relationship (QSPR) models, since the spline terms make it possible for modelling nonlinear relationships [22, 32]. The QSPR model developed via genetic functional approximation (GFA) is given in equation (9) as

$$
\text{Binding Energy} = -70.833 \times E \left( \frac{kJ}{mol} \right) + 106.348
$$
Predicted values (Binding Energy) | Actual values (Binding Energy)  
--- | ---  
-40.1715 | -29.796  
-92.7975 | -100.4  
-206.671 | -202.317  
-85.7529 | -92.88  

**Table 6:** Predicted and Actual values of the Binding Energy of Metal-Inhibitor Complex

This result is consistent with the correlation analysis of the binding energy of the inhibitor to the metal surface, hence confirming the significance of the total energy of the metals to the predictive ability of the model and important for improving the inhibitory property of clindamycin.

**Corrosion Rate Study Using Clindamycin on the Metal Plates Preparation of the metals**

Mild steel, Copper, Zinc plates and Aluminum were obtained from the Department of Metallurgical Engineering, Ahmadu Bello University, Zaria. The chemical composition in wt % for Mild steel was C = 0.181, Si = 0.056, Mn = 0.474, S = 0.039, P = 0.039, Ni = 0.078, Cr = 0.038 and the rest Fe, while Al contains Mn= 1.281, Pb = 0.064, Ti = 0.024, Cu = 0.51, Si = 0.381, Fe = 0.057 and Al = 96.55%. Mild Steel specimens of size 2 cm × 1 cm × 0.27 cm were used in weight loss experiments, while for the other metals the specimen size 5 cm × 4cm × 0.11cm were used. The concentration of HCl used for the experiments were 1M. Thread was tied to each of mild steel pieces for easy suspension in the media. Each coupon was mechanically polished using emery papers to remove scaling, surface contaminants and oxide film on the surface of the coupons. This was followed by employing the chemical cleaning procedure for removal of corrosion product from the surface of the metals [33,34]. The methods in C.1.1 (Al), C.2.1 (Cu), C.3.3 (Fe) and C.9.1. (Zn) described by ASTM G1-03-E (Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens) was used specifically for this study.

**Gravimetric Method**

Weight loss technique was employed in the experiment as follows. Each coupon was weighed using Analytical weighing balance and recorded as weight $W_1$. The coupon was suspended in a 100 cm$^3$ beaker using a thread. A 100 cm$^3$ of 1M HCl was introduced into reaction beakers. The experimental set-up was kept in the laboratory away from direct sunlight, while the time of exposure for each coupon was carefully noted. Each coupon was retrieved from the test medium in intervals of 24 hours. The corroded coupons were washed in 20%NaOH in 100 g/L zinc dust to stop the corrosion reaction and dried using acetone. The coupons were reweighed and the final weights, $W_2$ recorded. Weight losses, $\Delta W = W_1 - W_2$ were calculated. The inhibition efficiency % IE and surface coverage $\theta$ was determined by using the following equations:

$$\theta = \frac{W_o - W_i}{W_o}$$

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*Kenk Nanotec Nanosci 5:01-18(2019)*
Where \( w_i \) and \( w_0 \) are the weight loss value in presence and absence of inhibitor, respectively.

The corrosion rate (CR) is expressed as an increase in corrosion depth per unit time in (mg cm\(^2\) hr\(^{-1}\)). The corrosion rate equation is given as:

\[
CR = \frac{\Delta W}{At}
\]

Where \( \Delta W \) = weight loss of coupon, \( t \) = immersion time, and \( A \) = area of coupon.

**Effect of immersion time and temperature on corrosion rate**

The Figures below shows the plot of corrosion rate against immersion time. The corrosion rate increases as the immersion period is lengthen at a fixed concentration of the inhibitor (clindamycin), the changes seem to follow the trend for the weight loss of the metals in the absence of the inhibitor with a slight difference in aluminum.

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**Figure 8:** Variation of weight loss with immersion time for the corrosion of mild steel, aluminum, copper and zinc plate in blank solution of 1M HCl.
Figure 9: Variation of corrosion rate with immersion time for the corrosion of mild steel, aluminum, copper and zinc plate in solution of 1M HCl containing 0.1 g/L of the clindamycin inhibitor.

<table>
<thead>
<tr>
<th>Metal</th>
<th>%IE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>79.62</td>
</tr>
<tr>
<td>Cu</td>
<td>61.48</td>
</tr>
<tr>
<td>Al</td>
<td>40.74</td>
</tr>
<tr>
<td>Zn</td>
<td>44.21</td>
</tr>
</tbody>
</table>

Table 7: Percentage inhibition efficiency of clindamycin inhibitor on some metal surfaces in the presence of 1M HCl solution

The percentage (IE) inhibition efficiency greatly correlate with the value of the binding affinity of the inhibitor to the metal surface, the result though significantly confirms our theoretical study differ a bit when considering aluminum. Aluminum when oxidized exhibits a mild inert presence that prevents further corrosion of the metal surface. The high inhibition efficiency of the inhibitor to Fe and Cu, could be associated with the fact the these metals have empty or partial filled d-orbitals for which they could accept lone pair of
electron, hence increasing the stability of their newly formed bonds with the inhibitor.

Conclusion

The theoretical computed binding energy (kcal/mol) of clindamycin on the metals Al, Cu, Fe and ZnO were found to be (-92.880, -100.40, -202.317 and 29.796) kcal/mol respectively, this shows that inhibition efficiency of clindamycin will be best achieved when used on iron (Fe) and least when used on zinc (Zn). The quantum chemical parameters point out that this is because Zn having a completely filled d-orbitals limits the possibility of accepting lone pairs of electron from Sulphur, oxygen and nitrogen atoms present in clindamycin and hence have a low reactive index parameters in the adsorption of the inhibitor (clindamycin) on their surfaces.

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