Computational Approaches to the Corrosion Prevention Ability of Certain Significant Pharmaceutical Compounds Against Industrially Essential Metals

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Abstract

Although the ability of some medicinal compounds to prevent corrosion in metals under corrosive conditions has been investigated, more research is required before these results can be used in the industrial setting. Through theoretical work, this study examines the ability of ten pharmaceuticals, including Ibuprofen, Aspirin, Paracetamol, and others, to inhibit corrosion. The study's objective is to use quantum calculations to comprehend the atomic level process of metal corrosion prevention. Numerous parameters of the therapeutic molecules are calculated in the study, including dipole moment, global hardness, energy gap, and absolute electronegativity. According to the quantum studies, the adsorption process is greatly influenced by electron-rich species found in pharmaceutical drugs. The results of the study provide a solid basis for more experimental research.

Keywords: Metals, adsorption process, pharmaceutical chemical, corrosion prevention, and quantum calculations.

Introduction

In the metal business, corrosion is a key issue that causes serious financial losses and safety issues. For metals to be protected against corrosion, new and potent corrosion inhibitors must be developed. Flavonoids, carboxylic acids, and other natural products have been discovered to have remarkable corrosion-inhibitory characteristics in medicinal substances. However, a thorough understanding of their molecular interactions with metal surfaces is necessary for the design and development of novel, efficient corrosion inhibitors based on pharmaceutical compounds. Theoretical methods have become effective resources for forecasting the corrosion inhibition characteristics of pharmaceutical drugs, including molecular docking, molecular dynamics simulations, and density functional theory (DFT) computations. These computational techniques may aid in the development of fresh and efficient corrosion inhibitors by offering useful insights into the mode of action of pharmaceutical compounds as corrosion inhibitors. In this article, we examine the theoretical frameworks for computationally estimating the corrosion inhibitory capabilities of significant medicinal drugs against industrially significant metals. We also go through current research on the use of

pharmaceutical substances as corrosion inhibitors for metals including iron, steel, and aluminium. Our results indicate that the discovery and development of novel and efficient corrosion inhibitors based on pharmaceutical substances may be greatly aided by computational methods.

Corrosion prevention is mostly dependent on adsorption, and existing synthetic corrosion inhibitors are both expensive and hazardous. The creation of ecological corrosion inhibitors is becoming more and more popular as a solution to this problem. According to earlier studies, synthetic organic species may be replaced by medicinal compounds as non-toxic corrosion inhibitors for industrially significant metals in a variety of settings. To solve the practical concerns of employing pharmaceutical substances as corrosion inhibitors, further study is still required. One essential computational method used to research metal corrosion inhibition is quantum chemical calculations. In this work, we employed quantum chemical simulations to examine the effectiveness and mechanism of 10 pharmaceuticals, including aspirin, ibuprofen, and other drugs, in preventing metal corrosion. Our study offers insightful information about the impact of medicinal compound structures on corrosion prevention and the mechanism of corrosion inhibition. The research helps in the quest for brand-new, non-toxic corrosion inhibitors for different metals under corrosive circumstances, with possible industrial uses.

Materials and methods

Molecular structures: Ibuprofen, Aspirin, Paracetamol, Ranitidine, Acetaminophen, Warfarin, and Naproxen chemical structures. For the investigation of quantum parameters, phenazone, propylphenazone, and caffeine were obtained from the literature. The structure is taken in "mol" format for the analysis of quantum chemical characteristics.

Software and Quantum chemical calculation: The best technique to determine how well certain metals can withstand corrosion in various settings is using quantum chemical methods. To evaluate several quantum chemical parameters including ELUMO, EHOMO, I, chemical potential, A, chemical softness, chemical hardness, electrophilicity index, and electro negativity, the researchers employed cutting-edge software called ArgusLab.

Values for EHOMO and ELUMO are retrieved straight from the ArgusLab programme. The following relation may be used to determine the ionisation potential (I),

$I = -E_{HOMO}$

Following are the electron affinity (A) values that were determined using the E LUMO values:

$A = -_{ELUMO}$

The following criteria may be used to assess global hardness and electronegativity, respectively:

Electronegativity (χ) = I+A/2

Chemical hardness (η) = I-A/2

The equation below is used to compute the chemical softness (), also known as electron polarizability.

$\sigma = 1/\eta$

The following mathematical equation yields the chemical potential (),

$\mu = -\chi$

The following equation yields the electrophilicity index (),$\omega = \mu^2/\eta$

Table 1 provides thorough information on the adsorption components and double bonds that are present in medicinal compounds and are in charge of the adsorption process, which inhibits the dissolution reaction.

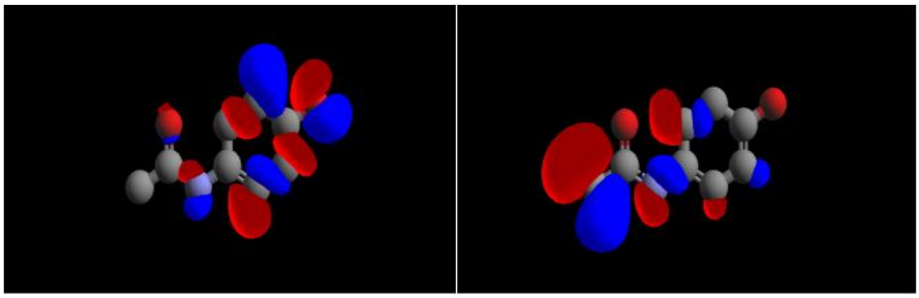
It is evident from Table 1 that the sole pharmaceutical molecule with S atoms is ranitidine. N atoms are found in the pharmaceutical substances caffeine, phenazone, propylphenazone, ranitidine, and acetaminophen. O atoms are present in every chemical that was analysed. Ibuprofen, Aspirin, Paracetamol, Acetaminophen, Warfarin, and Naproxen are among the substances investigated that have hydroxyl (OH) groups. The 10 pharmaceutical compounds all have double bonds. In general, we are aware that any chemical that has N, S, P, and O atoms as well as double bonds in its moieties will exhibit corrosion inhibition. Therefore, the general model of corrosion inhibitors is followed by all ten of the compounds we chose for our study.

Table-1: Detailed information about the medicinal compounds

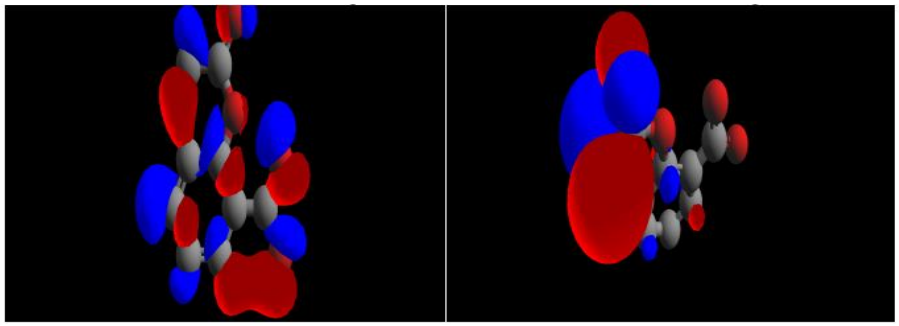
Compound name	Number of "S" atoms present	Number of "N" atoms present	Number of "O" atoms present	Number of "OH" groups present	Number of double bonds present
Ibuprofen	-	-	1	1	4
Aspirin	-	-	4	1	5
Paracetamol	-	1	2	1	4
Ranitidine	1	4	3	-	4
Acetaminophen	-	1	2	1	4
warfarin	-	-	4	1	9
Naproxen	-	-	3	1	6
Phenazone	-	2	1	-	5
Propylphenazone	-	2	1	-	5
Caffeine	-	4	2	-	4

Results and discussion

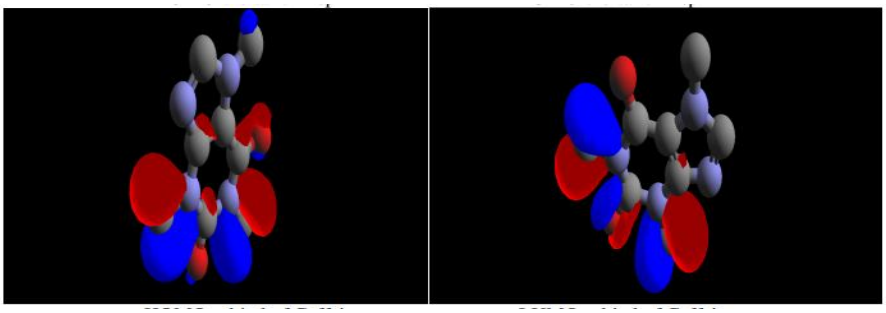
Acetaminophen, Aspirin, Caffeine, Ibuprofen, Naproxen, Paracetamol, Phenazone, Propylphenazone, Ranitidine, and Warfarin's HOMO and LUMO orbitals were shown in Figure 1.



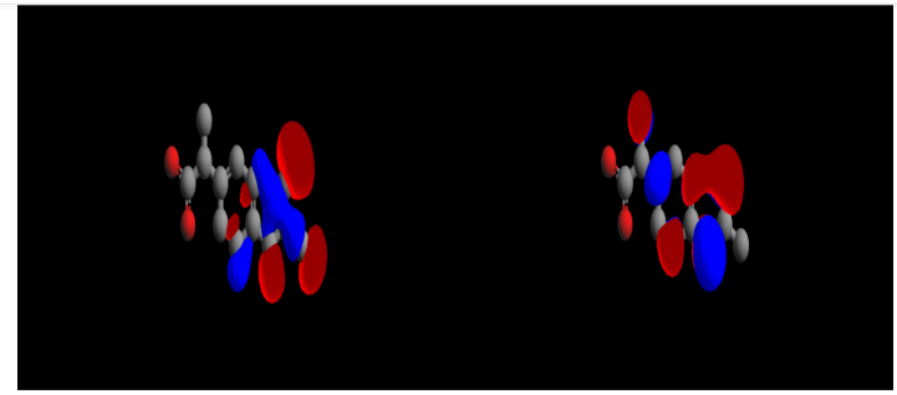
HOMO orbital of Acetaminophen LUMO orbital of Acetaminophen



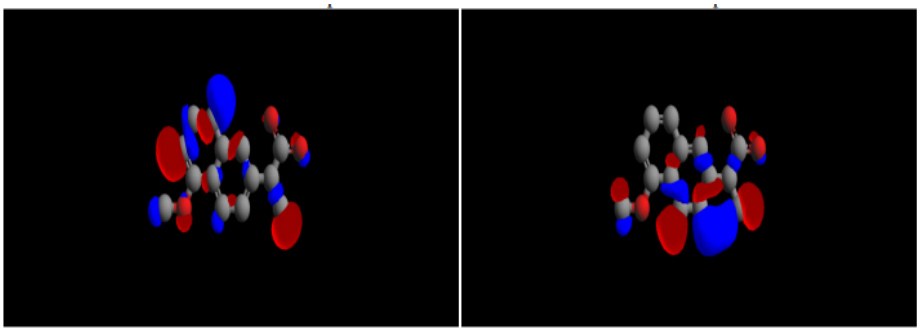
HOMO orbital of Aspirin LUMO orbital of Aspirin



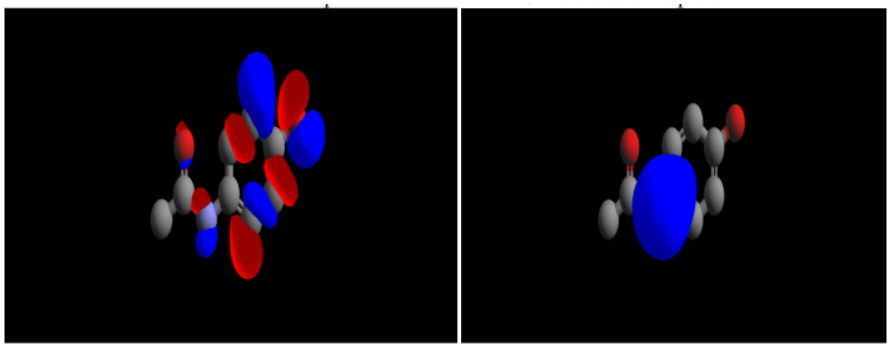
HOMO orbital of Caffeine LUMO orbital of Caffeine



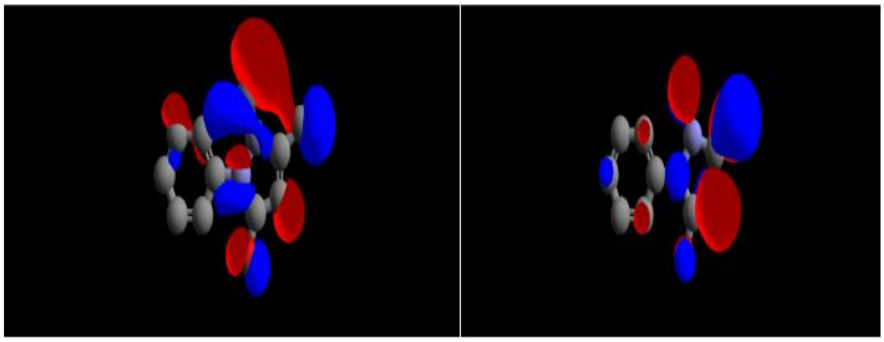
HOMO orbital of Ibuprofen LUMO orbital of Ibuprofen



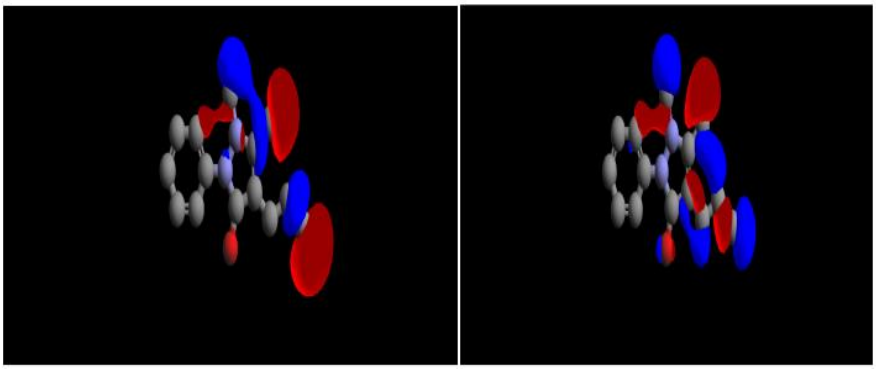
HOMO orbital of Naproxen LUMO orbital of Naproxen



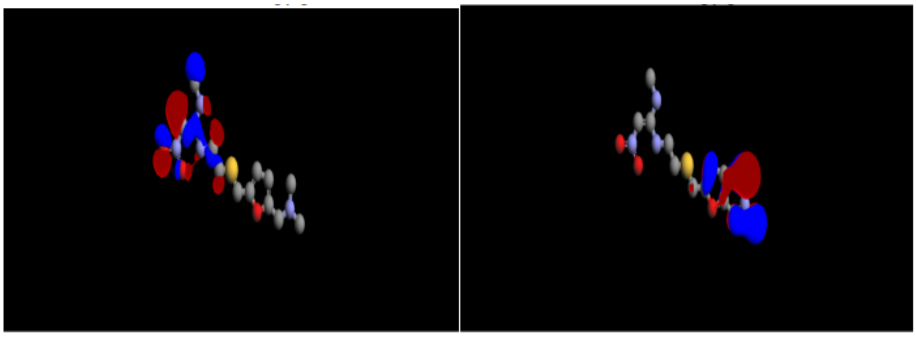
HOMO orbital of Paracetamol LUMO orbital of Paracetamol



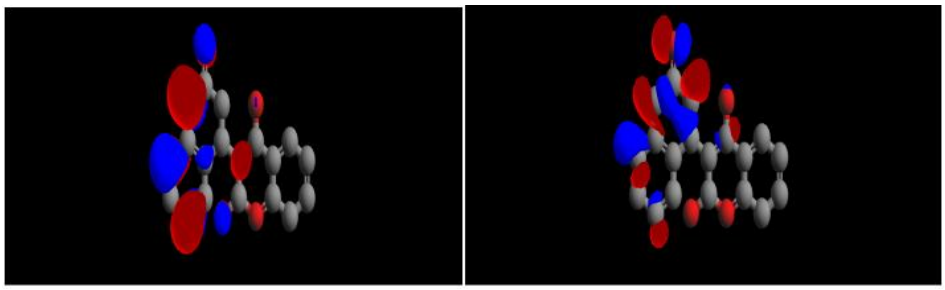
HOMO orbital of Phenazone LUMO orbital of Phenazone



HOMO orbital of Propylphenazone LUMO orbital of Propylphenazone



HOMO orbital of Ranitidine LUMO orbital of Ranitidine



HOMO orbital of Warfarin LUMO orbital of Warfarin

Figure-1: HOMO and LUMO orbital's of examined medicinal compound

To theoretically ascertain the electrical characteristics of the therapeutic species, E LUMO and E HOMO research are essential. Two colours are used to illustrate the orbital's negative and positive phases: red and blue. Red represents a reduction in electron density while blue represents an increase.

High EHOMO pharmaceutical substances often give electrons to metals, which have open, acceptible molecular orbitals. In our investigation, caffeine, naproxen, phenazone, propylphenazone, and ibuprofen had the highest E HOMO values. These materials are anticipated to adhere to the metal's surface and stop corrosion. These compounds' electron-rich constituents have an impact on their capacity to halt corrosion. Their reactivity is determined by the energy difference between the metal and the compounds. The compounds on the metal surface will be more reactive the narrower the energy gap, providing superior corrosion prevention.

Table-2: Quantum chemical parameters (by using PM3 method)

Name of medicinal compound	E_{HOMO} (eV)	E_{LUMO} (eV)	Energy gap (eV)	I	A	η	χ	σ	μ	ω
Acetaminophen	-3.499	3.974	7.474	3.499	-3.974	3.736	-0.237	0.267	0.237	0.00751
Aspirin	-9.580	-3.240	6.340	9.580	3.240	3.170	6.410	0.315	-6.410	6.48075
Caffeine	-10.79	-3.455	7.337	10.792	3.455	3.6685	7.123	0.272	-7.120	6.909
Ibuprofen	-9.703	-2.857	6.846	9.703	2.857	3.423	6.28	0.292	-6.280	5.760
Naproxen	-10.31	-2.367	7.945	10.312	2.367	3.972	6.339	0.251	-6.339	5.058
Paracetamol	-3.499	3.972	7.471	3.499	-3.972	3.735	-0.236	0.267	0.236	0.00748
Phenazone	-10.11	-2.965	7.154	10.119	2.965	3.577	6.542	0.279	-6.542	5.990
Propylphenazone	-9.855	-3.945	5.91	9.885	3.945	2.955	6.900	0.338	-6.90	8.0558
Ranitidine	-9.581	-2.770	6.811	9.5814	2.770	3.4057	6.1757	0.293	-6.175	5.607
Warfarin	-8.977	-2.809	6.168	8.977	2.809	3.084	5.893	0.324	-5.893	5.6301

According to the energy gap idea, the reactivity order is as follows: Propylphenazone, Warfarin, Aspirin, Ranitidine, Ibuprofen, Phenazone, Caffeine, Paracetamol, Acetaminophen, and Naproxen are some examples of medications.

Due to its strong reactivity in comparison to other pharmaceutical compounds, propylphenazone is predicted to exhibit the greatest corrosion inhibition property on the surface of industrial metals based on energy gap values. Propylphenazone has five double bonds, two nitrogen atoms, one oxygen atom, and wants to contact strongly with electrode (metal) surfaces in corrosive ions, which makes it a great corrosion inhibitor.

High I values indicate that an organic compound is very stable and chemically inert. The great reactivity of the medicinal chemical is shown by the low I values. Low I levels indicate effective protection.

According to the I values, the therapeutic substances react in the following order: Acetaminophen, Naproxen, Warfarin, Aspirin, Ranitidine, Propylphenazone, Propylphenazone, Phenazone, and Caffeine are some examples of common medications.

To assess the reactivity and stability of therapeutic substances, softness and hardness are essential characteristics. When compared to other pharmaceutical chemicals, propylphenazone has the lowest hardness value (2.955) and the second-highest softness value. Typically, in concentrated corrosive solutions, the organic compound with low hardness and high softness value demonstrates the excellent inhibitory property on metal surfaces. The electrophilic or nucleophilic character of the medicinal molecule is shown by electrophilicity values.

Low values indicate that the molecule acts as a strong nucleophile, whereas high values indicate that the pharmaceutical chemical acts as a strong electrophile. The strongest electrophile is propylphenazone, which has a high electrophilicity value; the strongest nucleophile is paracetamol, which has a low electrophilicity value. (Table-2)

Conclusion

According to the E HOMO value calculated using the quantum chemical approach, the molecules of caffeine, naproxen, phenazone, propylphenazone, and ibuprofen significantly adsorb on the surface of the metal. Propylphenazone was predicted to have strong anticorrosive properties based on energy values because of its high reactivity. Hardness and softness characteristics are also very supportive of propylphenazone's improved ability to stop corrosion. The findings of quantum chemistry investigations show that all of the pharmaceutical substances under investigation have anticorrosion properties; however the degree of protection varies. These findings provide a solid framework for the experimental exploration of corrosion inhibitors needed to stop the process of metal breakdown.

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