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THEORETICAL ANALYSIS OF BINAHONG LEAF EXTRACT AS CORROSION INHIBITOR USING THE DFT METHOD

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ABSTRACT

Binahong leaf extract has been experimentally tested containing several compounds that are effective used as corrosion inhibitors. Further computational chemical research was conducted to determine the interaction of the compounds contents, including vitexin, ursolic acid and p-coumaric acid with the iron using the Density Functional Theory (DFT) method based on B3LYP/6-31G. Quantum chemical parameters from optimization results include E_{HOMO}, E_{LUMO}, dipole moment, energy gap (ΔE), electronegativity (χ), ionization potential (I), electron affinity (A), hardness (η), softness (σ), electrophilicity (ω) and nucleophilicity (ε). The interaction strength parameters of the inhibitor with Fe atom, namely charge transfer (ΔN), interaction energy ($\Delta\psi$) dan back-donation energy (ΔE_{b-d}), indicate that ursolic acid is the best inhibitor molecule. The interaction of inhibitor with Fe (100) seen from the energy of adsorption (E_{ads}) and the bonding energy ($E_{binding}$) suggests that among the three main contents of plant leaf extract, ursolic acid has the highest value of 111.92 kJ/mol with a bond length value of Inh-Fe of 1.91 Å. Binding length data and binding energy indicate that the interaction that occurs is a chemical interaction.

INTRODUCTION

Corrosion is a natural phenomenon in which metals and alloys try to return to their more stable thermodynamic forms, by chemical attack or by reaction with their environment. Corrosion is known to be dangerous to the environment and also to human well-being. Corrosion effects can be considered a vital situation that requires proper prevention as they

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can be a threat to economic impact, material conservation and security in various engineering applications (Zuliana et al., 2021). Different methods can be used to reduce the corrosion level, one of which is the use of corrosion inhibitors. They reduce corrosions mainly by increasing or decreasing anode and/or cathode reactions and reducing the diffusion rate for reagents to the metal surface and the electrical resistance of the surface (Muthukrishnan et al., 2019).

Organic inhibitors are an alternative to corrosion control because they are biodegradable and do not contain heavy metals or other toxic compounds (Belghiti et al., 2018). Organic molecules containing O, N, and/or S atoms can be used as an effective corrosion inhibitor. Generally, this happen because they can be absorbed on the metal surface through several active groups such as heteroatoms, triple bonds or aromatic rings. Most organic inhibitors reduce the corrosive rate by adsorption on the substrate surface with atomic sequence O < N < S < P (Guo et al., 2018). There are many studies that show the use of leaves, fruits, bark and seed as corrosion inhibitor, such as kecapi leaf extract (Wahyuni et al., 2022) , melinjo bark extract (Emriadi et al., 2018) and kweni seed extract (Stiadi et al., 2020).

Previously, experiments had been carried out on the extracts of binahong (*Anredera cordifolia* (Ten.) Steenis) leaf that were effectively used as corrosion inhibitor (Putri, 2018). It is a herbal plant that has been studied for its benefits in the treatment of wounds and diseases because it has high antioxidant activity. Binahong leaf extract contains several major compounds including vitexin (Harahap et al., 2019), ursolic acid (Mulia et al., 2019) and p-coumaric acid (Fachriyah et al., 2019).

Currently, computer modeling techniques have been widely used to study metal corrosion inhibition. The computational methods have proven to be quite useful in determining the structure of inhibitor molecules and clarifying their electronic properties and reactivity. Density functional theory (DFT) is one method which is able to study the interaction between metal surfaces and inhibitors. DFT used to examine the electronic configuration, primarily the lowest energy state, of complex systems such as atoms, molecules, and their condensed forms. The primary objective is to substitute the many-body electronic wave function with the electronic density, which serves as the fundamental quantity (Abeng et al., 2022).

Several theoretical studies related to corrosion inhibitors, in particular using the DFT method, have been carried out. One of them is against the vitexin compound which is the compounds contained in the leaf extracts of binahong. According to (Ayuba & Umar, 2021), vitexin is potentially a good corrosion inhibitor and can be adsorbed on aluminum surfaces through physical adsorption mechanisms. Therefore, this study aims to further analyze the interactions between the compounds contained in the leaves of strawberries as a corrosion inhibitor on iron in a computerized way.

RESEARCH METHODS

Molecule Structure

The 3D structure of vitexin molecules, ursolic acid and p-coumaric acid is obtained from the PubChem site (https://pubchem.ncbi.nlm.nih.gov/) as shown in Figure 1. Next, optimized using Gaussian 16W software with DFT method and based on B3LYP/6-31G.

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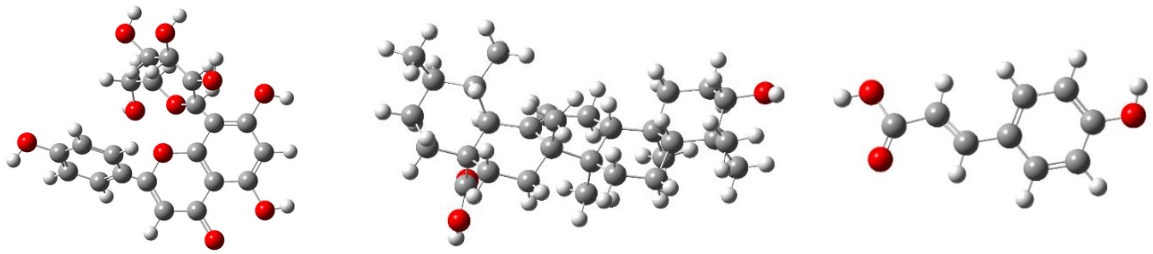

a) b) c)

Figure 1. 3D Structure a) Vitexin b) Ursolic acid c) p-coumaric acid (atomic color: grey = carbon, red = oxygen, white = hydrogen)

Quantum Chemical Parameters

Orbital theory is useful for predicting the adsorption of inhibitor molecules and their interactions with metals. HOMO energy (E_{HOMO}) indicates the ability of a molecule to donate electrons to an acceptor. E_{HOMO} tends to donate electrons to acceptors with empty low-energy molecular orbitals. While LUMO energy (E_{LUMO}) shows the ability to accept electrons from a molecule. Frontier molecular orbitals (FMO) can provide theoretical results easily, according to the energy gap values between E_{HOMO} and E_{LUMO} (Radhi et al., 2020). The gap energy (ΔE) value is expressed by equation (1):

$$\Delta E = E_{LUMO} - E_{HOMO} \quad (1)$$

The ionization potential (I) and electron affinity (A) parameters are calculated using Koopman's theorem. Ionization potential can be defined as the amount of energy required by a molecule to release an electron. Electron affinity is defined as energy released when a proton is added to a system (Hadisaputra et al., 2017). The value show in equations (2) and (3) below:

$$I = -E_{HOMO} \quad (2)$$

$$A = -E_{LUMO} \quad (3)$$

Hardness and softness parameters are used to predict the reactivity of a molecule. Hardness is the reluctance of a system to released electrons, while global softness (σ) is the inverse of global hardness (Obi-Egbedi & Ojo, 2015). The hardness and softness values can be expressed in equations (4) and (5) below:

$$\eta = \frac{I - A}{2} \quad (4)$$

$$\sigma = \frac{1}{\eta} \quad (5)$$

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Electronegativity (χ) shows the ability of a molecule to attract electrons (Yao Silvère DIKI et al., 2019). The electronegativity equation is like equation (6) below:

$$\chi = \frac{I + A}{2} \quad (6)$$

The electrophilicity index (ω) indicates the ability of a molecules to accept electrons, while nucleophilicity (ε) is the inverse of electrophilicity which indicates the tendency of molecules to donate or share electrons (Ayuba & Umar, 2021). Electrophilicity and nucleophilicity values are calculated using equations (7) and (8) below:

$$\omega = \frac{\chi^2}{2\eta} \quad (7)$$

$$\varepsilon = \frac{1}{\omega} \quad (8)$$

The interaction of Fe and inhibitor shows that electrons will move from lower electronegativity (inhibitor) to higher electronegativity (Fe), until the chemical potential becomes the same (Arthur et al., 2019). The volume of electrons carried (ΔN) calculated by equation (9) as below:

$$\Delta N = \frac{\chi Fe - \chi inh}{2(\eta Fe + \eta inh)} \quad (9)$$

Interaction energy (Δψ) is a value that shows the strength of the bond between the inhibitor and the metal (Guo et al., 2018). The interaction energy can be calculated using the following equation (10):

$$\Delta\psi = \frac{(\chi Fe - \chi inh)^2}{4(\eta Fe + \eta inh)} \quad (10)$$

Back-donation energy ($\Delta E_{b\text{-}d}$) shows the existence of a bond between the inhibitor and the metal which is formed through the sharing of electrons from the metal to the inhibitor (reverse donation) (Huong et al., 2019). The back-donation energy value is expressed by the following equation (11):

$$\Delta E_{b\text{-}d} = -\frac{\eta}{4} \quad (11)$$

Adsorption energy (E_{ads}) is a parameter that shows the strength of a metal to absorb inhibitors. Meanwhile, binding energy ($E_{binding}$) is the strength of an inhibitor to bind to metal ions (Mi et al., 2015). The adsorption and bond energy are calculated using equations (12) and (13) as below:

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$$E_{ads} = E_{kompleks} - (E_{Fe} + E_{inhibitor}) \quad (12)$$

$$E_{binding} = -E_{ads} \quad (13)$$

RESULTS AND DISCUSSION

Contour HOMO-LUMO

After optimization, obtained electron density distribution HOMO and LUMO that can predict the adsorption center and inhibitor molecular interaction center. Results of optimization of the geometry of the molecules vitexin, ursolic acid and p-coumaric acid can be seen in Figure 2.

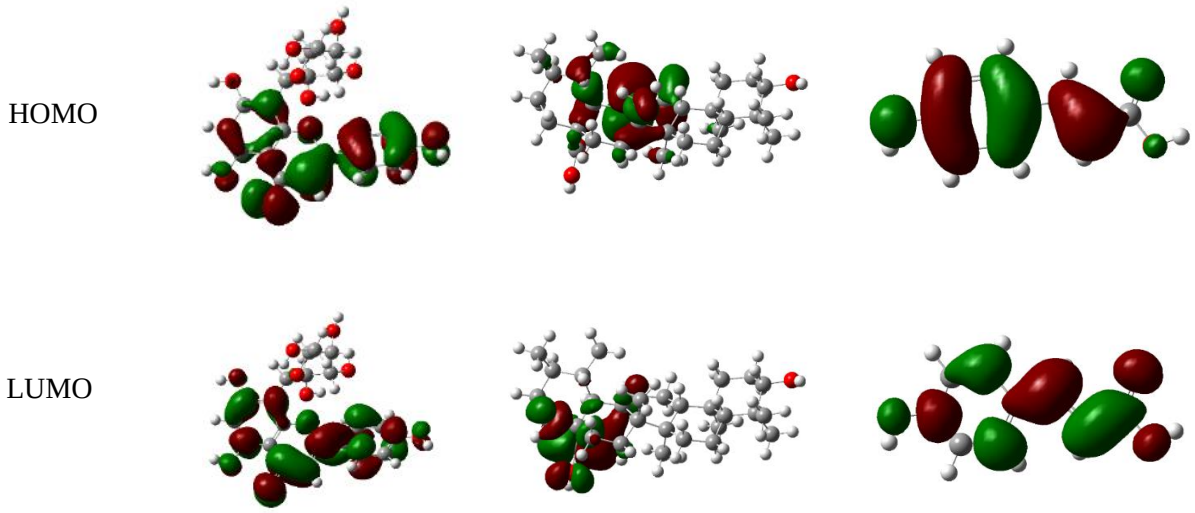

Figure 2. Contour HOMO and LUMO of the contents of binahong leaf extract (a) Vitexin (b) ursolic acid (c) p-coumaric acid

Frontier orbital theory is useful in predicting adsorption centers inhibitor molecules, so it can be known where the inhibitor interacts with the metal (Obot & Obi-Egbedi, 2010). From Figure 2, it can be observed that both HOMO and LUMO of the three molecules are distributed on the oxygen atoms and the aromatic rings of the molecule, this shows their tendency to participate in the donor and electron aseptor processes The HOMO orbital is relatively more distributed on the oxygen atom compared to the aromatic ring of the inhibitor molecule, this indicates the better ability of the oxium atom to contribute electrons compared with the aromatical ring, this is due to the availability of free electron pairs.

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Table 1. E_{HOMO}, E_{LUMO}, ΔE_{gap} dan E_{total} values of the inhibitor

Inhibitor	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE_{gap} (eV)	E_{tot} (Hartree)
Vitexin	**-5,94**	-1,42	4,52	**-1563,97**
Ursolic acid	-6,08	-0,24	5,83	-1397,40
p-coumaric acid	-6,15	**-1,89**	**4,26**	-573,28

The molecular orbital energy of the binahong leaf extract content is presented in Table 1. It can be observed that the vitexin compound is more readily able to donate electrons because it has a higher E_{HOMO} value. While p-coumaric acid has the smallest E_{LUMO} value among the other two inhibitors, this indicates that the molecule can easily receive electrons from the metal surface and cause stronger adsorption.

From the E_{HOMO} and E_{LUMO} values obtained, the gap energy value (ΔE) can be determined, which also determines the reactivity and stability of the molecule against the metal surface. The energy gap is the difference in the energy level between the HOMO and LUMO energies. The larger the ΔE value, the more stable and less reactive it becomes, because it requires a large amount of energy to experience electron excitation from HOMO to LUMO. By contrast, when the value of ΔE is smaller, less energy is needed to experience electronic excitation (Radhi et al., 2020). From the optimization results, p-coumaric acid has better stability and reactivity between the other two compounds.

Molecular inhibitor optimization produces total energy (E_{tot}) which also shows the stability of a molecule. The smaller the E_{tot} value, indicates that the molecular stability is reduced, so it is easier to adsorb on the metal surface. This will result in a molection's ability to inhibit more strongly (Belghiti et al., 2019). From the optimization results obtained, the vitexin compound has a lower stability than ursolic acid and p-coumaric acid because it has the smallest total energy value.

Quantum chemical parameters

HOMO and LUMO energy values optimized using the DFT method of the crop leaf extract content can be used to calculate a variety of chemical quantum parameters as shown in Table 2 below.

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Table 2. Quantum chemical parameter values of inhibitor compounds

Parameter	Vitexin	Ursolic acid	p-coumaric acid
I (eV)	**5,94**	6,08	6,15
A (eV)	1,42	0,24	**1,89**
χ (eV)	3,68	**3,16**	4,02
η (eV)	2,26	2,92	**2,13**
σ (eV^{-1})	0,44	0,34	**0,47**
ω (eV)	3,00	**1,71**	3,80
ε (eV^{-1})	0,33	**0,58**	0,26

In Table 2, it can be observed that vitexin compounds have smaller ionization potential values, so it is easier to release electrons to the Fe atom. Meanwhile, p-coumaric acid is a molecule that is harder to receive electrons than a metal because it has a larger electron (A) affinity value.

The ursolic acid molecule has the lowest electronegativity (χ) among the other two inhibitors, so it is not easy to receive electrons from the metal. Meanwhile, p-coumaric acid has better strength values (η) and softness (σ), which indicates that it has a good tendency to react with metals.

Electrophilicity (ω) indicates the ability of a molecule to receive electrons. It's combined with the definition of electronegativity. Thus, ursolic acid molecules have the lowest values of electronegativity and electrophilicity. Nucleophilicity (ε) is an inverse of electrophilicity that represents the molecular tendency to donate electrons. From the results of the optimization in Table 2, it is noted that the value of the parameter nucleophilicity of ursolic acid is the highest. It suggests that ursolic acid has the ability to donate electrons to metals.

Electrostatic Surface Potential (ESP)

Electrostatic Surface Potential (ESP) shows the electropositive and electronegative regions of a molecule. The red color shows the most electronegative area, while the blue color shows the most electropositive area (Ibrahim et al., 2023).

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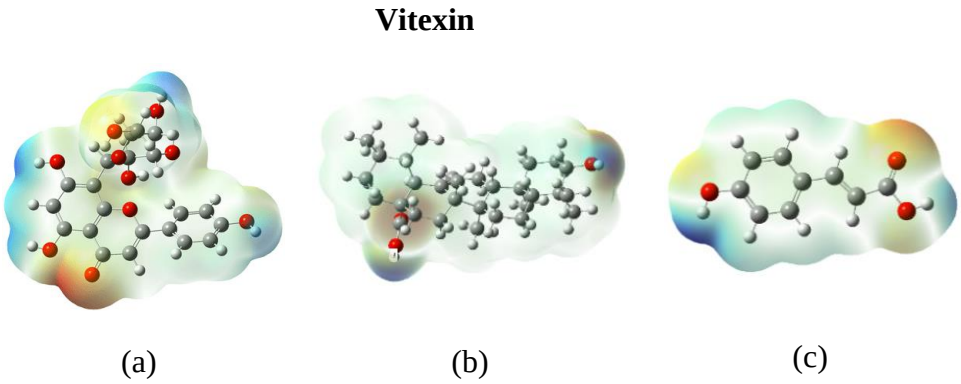

Figure 3. ESP content of binahong leaf extract (a) Vitexin (b) ursolic acid (c) p-coumaric acid

From the ESP results in Figure 3, it can be observed that the most electronegative areas are around the oxygen atom, both in the -OH group and in the -C=O group. This indicates that the Fe atom can most easily bond to the lone pair of electrons on the O atom.

Mulliken Charge Density

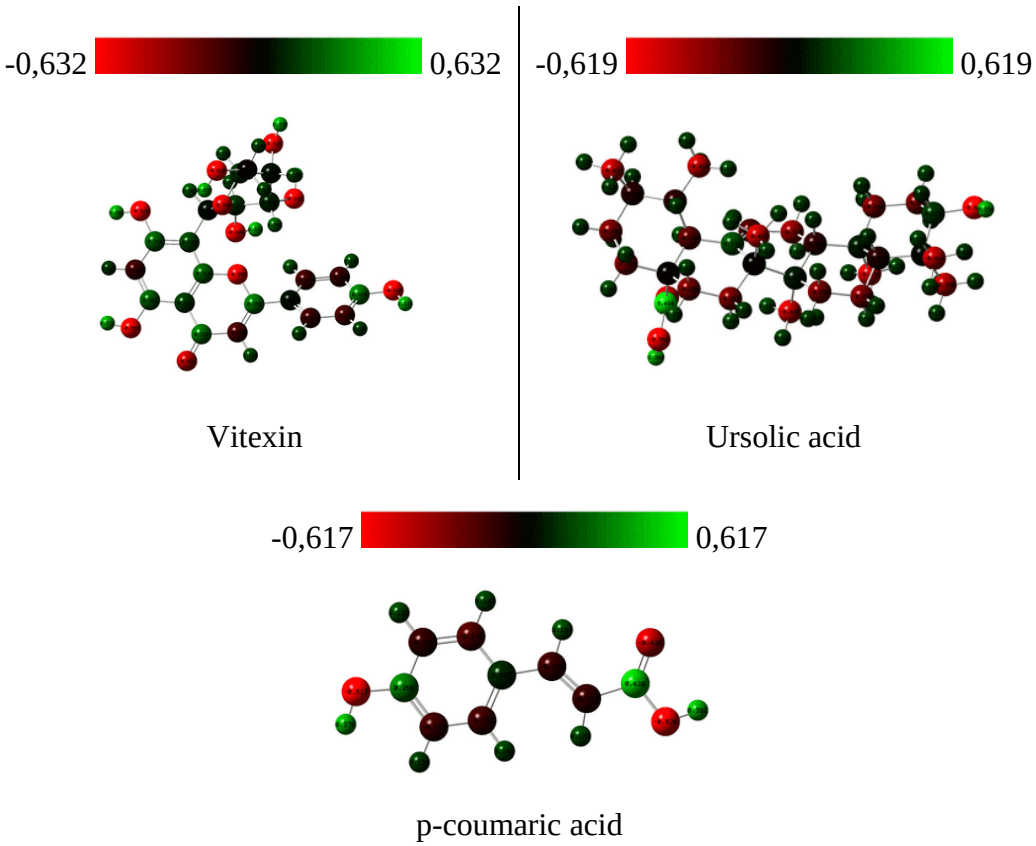

Figure 4. Mulliken density of binahong leaf extract

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The mulliken density value of the binahong leaf extract content is shown in Figure 4. Both vitexin, ursolic acid and p-coumaric acid molecules have more than one negative atomic charge value on the oxygen atom. This indicates that the O atom has the greatest ability to bond with the metal surface. The more negative the charge value of an atom, the greater the atom's ability to be adsorbed on the metal surface and the easier it will be for inhibitor molecules to donate electrons to the metal surface (Obi-Egbedi & Ojo, 2015). The most negative charge value for the O atom, namely -0.632, in the vitexin compound is located at the O43 atom. Meanwhile, in the compounds ursolic acid and p-coumaric acid, the most negative charge on the O atom is located on the O1 atom with values of -0.619 and -0.17.

Parameters of Inhibitor Interaction Strength with Fe Atom

The reactivity parameters of inhibitors with Fe atoms can be determined by the value of charge transfer (ΔN), interaction energy (Δψ), back-donation energy (ΔEb-d) and dipole moment as presented in Table 3.

Table 3. Calculated values of inhibitor reactivity parameters with Fe atoms

Inhibitor	ΔN (eV)	Δψ (eV)	ΔE_{b-d} (eV)	Dipole moment (Debye)
Vitexin	0,11	0,04	-0,57	**4,77**
Ursolic acid	**0,16**	**0,10**	**-0,73**	2,88
p-coumaric acid	0,06	0,01	-0,53	3,69

From Table 3, it can be concluded that the ursolic acid compound has better reactivity parameter values than other compounds. This can be seen from the highest value of charge transfer and interaction energy, as well as the lowest value of back-donation energy.

Inhibitor molecules have a strong tendency to donate electrons to empty metal orbitals. Based on the charge transfer values in Table 3 above, ursolic acid has a greater ability to donate electrons because it has a higher ΔN value. Interaction energy (Δψ) is a value that shows the strength of the bond between the inhibitor molecule and the metal (Guo et al., 2018). Among the binahong leaf extract contents that have been tested, ursolic acid has a higher Δψ value, so it has a strong bond when interacting with metals. Back-donation energy (ΔE_{b-d}) is another important parameter that describes the interaction of inhibitor molecules with the metal surface. Therefore, based on Table 3 above, the most stable molecule is the ursolic acid molecule which has the smallest ΔE_{b-d} value.

The dipole moment is another important electronic parameter that is the result of the uniform charge distribution on the atom and the distance between two bonded atoms. High dipole moment values are reported to increase adsorption and therefore inhibition by influencing the transport process through the adsorbed layer, inhibition efficiency increases with high dipole moment values (Radhi et al., 2020). Based on the data in Table 3, vitexin has the highest dipole moment value compared to the other two inhibitors.

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Inhibitor interaction with Fe(100)

In this research, Fe crystals (100) were used to analyze the interaction of inhibitor molecules as a corrosion inhibitor on iron. Based on the mulliken density that has been studied previously, one of the Fe atoms will bond with the oxygen atom which has the smallest electronegativity value.

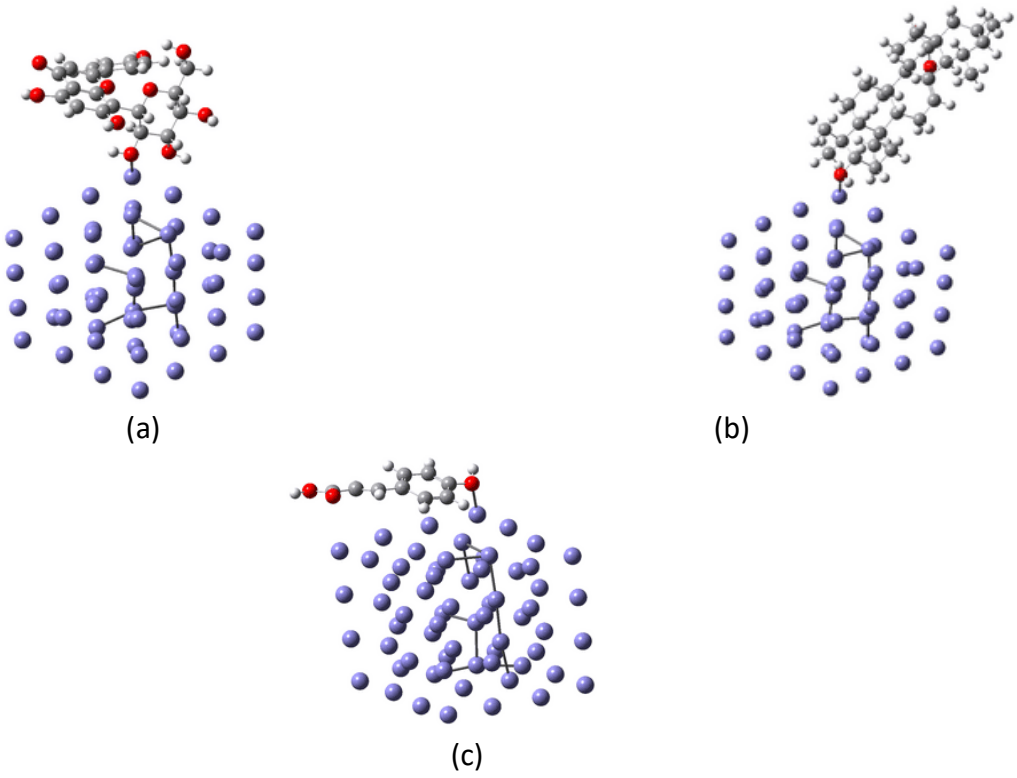

Figure 5. Interaction of inhibitors with Fe (100) (a) Vitexin (b) ursolic acid (c) p-coumaric acid

To determine the interactions that occur between molecules and inhibitors, optimization is carried out on each molecule, the Fe crystal and the combination between the molecule and the Fe crystal. Optimization was carried out using the Gaussian 16 W program with the Molecular Mechanics method, to obtain Fe energy values, inhibitor energy values and complex energy values. The energy obtained from the optimization process is useful for calculating the E_{ads}, $E_{binding}$ values and bond lengths between Fe and O atoms as shown in Table 4.

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Table 4. Interaction values of inhibitors with Fe (100)

Inhibitor	E_{ads} (kJ/mol)	$E_{binding}$ (kJ/mol)	r Fe-O (Å)
Vitexin	107,10	-107,10	**1,91**
Ursolic acid	**111,92**	**-111,92**	1,91
p-coumaric acid	19,30	19,30	1,93

Adsorption energy is a parameter that shows the strength of a metal to absorb an inhibitor, while bond energy is the strength of an inhibitor to bind to a metal. A negative value for Ebinding indicates that the reaction is exothermic. Among the three main contents of binahong leaf extract, ursolic acid showed the highest adsorption energy, namely 111.92 kJ/mol.

The bond distance between the inhibitor molecule and Fe also influences the reactivity of a molecule as an inhibitor. The smaller the bond distance, the stronger the bond between the inhibitor and the metal. When this distance is less than 3.5 Å, it is chemical adsorption (Huong et al., 2020). From the results obtained, the bond length of the inhibitor compounds shows almost the same value and the interactions that occur are chemical interactions.

CONCLUSION

Based on the results of optimizing the content of binahong leaf extract using the DFT method and the B3LYP/6-31G basis set, the E_{HOMO}, E_{LUMO} and dipole moment values were obtained. The obtained E_{HOMO} and E_{LUMO} values are used for calculating quantum chemical parameters such as gap energy (ΔE), electronegativity (χ), ionization potential (I), electron affinity (A), hardness (η), softness (σ), electrophilicity (ω) and nucleophilicity (ε). Based on the parameters of the interaction strength of the inhibitor with the Fe atom, such as charge transfer (ΔN), interaction energy (Δψ), and back-donation energy (ΔE_{b-d}), ursolic acid is the best inhibitor molecule among other inhibitor molecules. Meanwhile, the interaction of the inhibitor with Fe (100) shows that among the three main contents of binahong leaf extract, ursolic acid has the highest adsorption energy (E_{ads}) and binding energy ($E_{binding}$), namely 111.92 kJ/mol with a bond length value of Inh- Fe 1.91 Å. The bond energy and bond length data show that the interaction between the inhibitor and the Fe molecule is a chemical interaction.

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