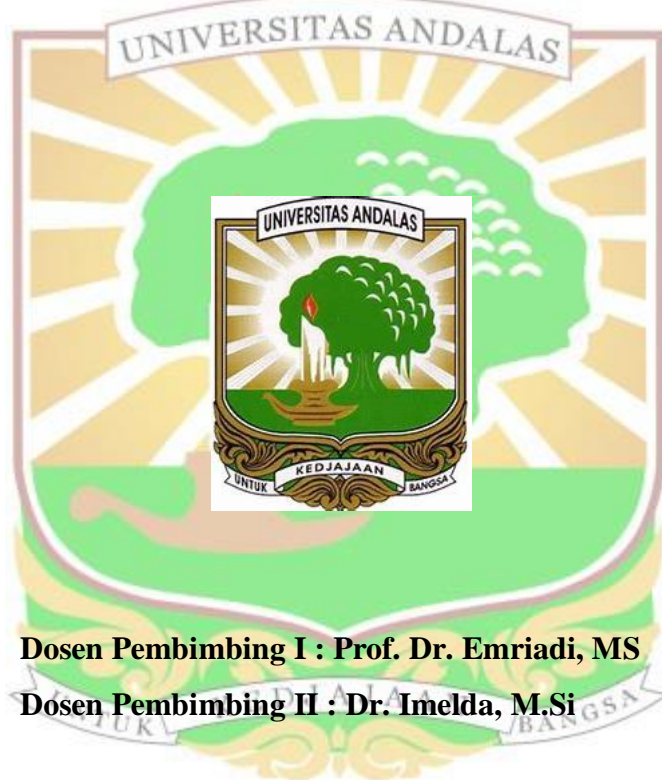


**ANALISIS TEORITIK KANDUNGAN EKSTRAK DAUN BINAHONG
(*Anredera cordifolia* (Ten.) Steenis) SEBAGAI INHIBITOR KOROSI
MENGUNAKAN METODE *DENSITY FUNCTIONAL THEORY* (DFT)**

TESIS

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Analisis Teoritik Kandungan Ekstrak Daun Binahong (*Anredera cordifolia* (Ten.) Steenis) sebagai Inhibitor Korosi Menggunakan Metode *Density Functional Theory* (DFT)

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Abstrak

Penelitian kimia komputasi dilakukan untuk mempelajari inhibisi korosi besi oleh senyawa vitexin, asam ursolat, asam p-kumarat, vitexin-2''-O-xyloside, vitexin-2''-O-rhamnoside dan vitexin-2''-O-glucoside menggunakan metode *Density Functional Theory* (DFT) dengan basis set B3LYP/6-31G. Parameter yang diperoleh dari hasil optimasi adalah E_{HOMO} , E_{LUMO} , momen dipol, energi gap (ΔE), elektronegativitas (χ), potensial ionisasi (I), afinitas elektron (A), hardness (η), softness (σ), elektrofilitas (ω) dan nukleofilitas (ϵ). Parameter kekuatan interaksi inhibitor dengan atom Fe yaitu transfer muatan (ΔN), energi interaksi ($\Delta \psi$), dan energi *back-donation* ($\Delta E_{\text{b-d}}$). Hasil perhitungan menunjukkan asam ursolat merupakan molekul inhibitor terbaik dalam kondisi tanpa pelarut, pelarut air dan terprotonasi. Interaksi inhibitor dengan kristal Fe (100) dilihat dari energi adsorpsi (E_{ads}) dan energi ikatan (E_{binding}) menunjukkan bahwa di antara tiga kandungan utama ekstrak daun binahong, asam ursolat memiliki nilai paling besar yaitu 111,92 kJ/mol dengan nilai panjang ikatan Inh-Fe 1,91 Å. Sementara pada golongan senyawa vitexin, vitexin-2''-O-glucoside memiliki nilai paling besar yaitu 122,53 kJ/mol dengan nilai panjang ikatan Inh-Fe 1,92 Å. Data panjang ikatan dan energi ikatan menunjukkan bahwa interaksi antara inhibitor dan Fe adalah interaksi kimia.

Kata Kunci: *Anredera cordifolia* (Ten.) Steenis, Inhibitor korosi, DFT



Theoretical Analysis of Binahong Leaf Extract (*Anredera cordifolia* (Ten.) Steenis) as Corrosion Inhibitor Using Density Functional Theory Method (DFT)

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Abstract

Computational chemical research was conducted to study the corrosion inhibition of iron by vitexin, ursolic acid, p-coumaric acid, vitexin-2''-O-xyloside, vitexin-2''-O-rhamnoside and vitexin-2''-O-glucoside using the Density Functional Theory (DFT) method with the B3LYP/6-31G basis set. The parameters obtained from the optimization results are E_{HOMO} , E_{LUMO} , dipole moment, gap energy (ΔE), electronegativity (χ), ionization potential (I), electron affinity (A), hardness (η), softness (σ), electrophilicity (ω) and nucleophilicity (ϵ). The parameters for the interaction strength of the inhibitor with Fe atoms are charge transfer (ΔN), interaction energy ($\Delta\psi$), and back-donation energy ($\Delta E_{\text{b-d}}$). The calculation results show that ursolic acid is the best inhibitor molecule in solvent-free, aqueous and protonated conditions. The interaction between the inhibitor and Fe crystal (100), as indicated by adsorption energy (E_{ads}) and binding energy (E_{binding}) shows that among the three main components of binahong leaf extract, ursolic acid has the highest value at 111,92 kJ/mol with an Inh-Fe bond length of 1,91 Å. Meanwhile, among the vitexin compounds, vitexin-2''-O-glucoside has the highest value at 122,53 kJ/mol with an Inh-Fe bond length of 1,92 Å. The bond length and binding energy data indicate that the interaction between the inhibitor and Fe is a chemical interaction.

Keywords: *Anredera cordifolia* (Ten.) Steenis, Corrosion inhibitor, DFT

