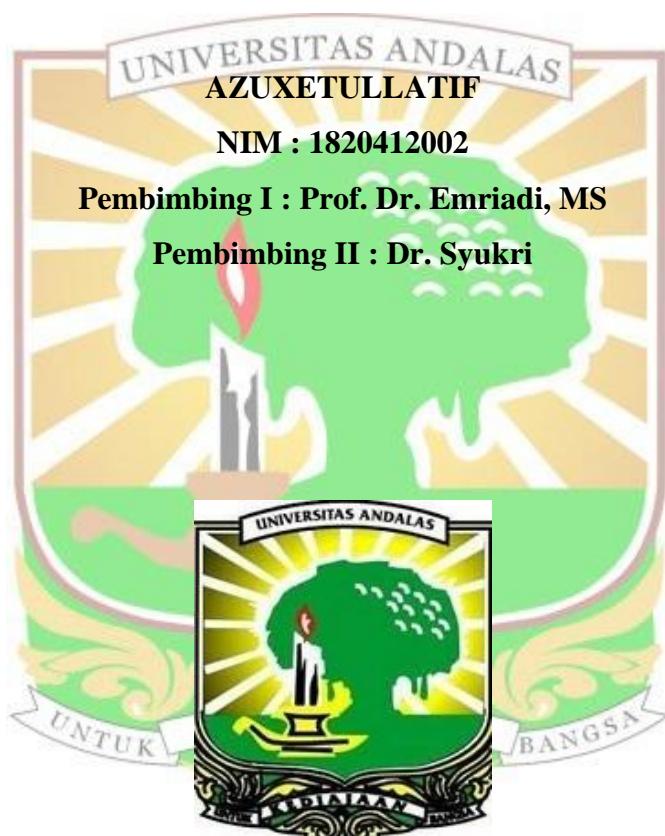


**MEMPELAJARI SENYAWA MIRISETIN DAN TURUNANNYA
SEBAGAI INHIBITOR KOROSI DENGAN METODE
*DENSITY FUNCTIONAL THEORY (DFT)***

TESIS



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ABSTRACT

A THEORETICAL STUDY OF THE CORROSION INHIBITION EFFECT OF MYRICETIN AND ITS DERIVATIVES ON MILD STEEL USING DENSITY FUNCTIONAL THEORY

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Computational research has been investigated on inhibition corrosion of myricetin (A), myricitrin (B), myricetin 3'glucoside (C), and myricetin 3-alpha-arabinofuranoside (D) using Density Functional Theory (DFT) at the B3LYP/6-31G (d, p) using a Gaussian program. The parameters obtained from the optimization result of quantum chemistry are calculated E_{HOMO} , E_{LUMO} and dipole moment (μ). From the value of E_{HOMO} and E_{LUMO} obtained then calculated energy gap (ΔE), dipole moment (μ), ionization potential (I), electron affinity (A), electronegativity (χ), hardness (η), softness (σ), transferred electrons (ΔN), electrophilicity (ω), interaction energy (ΔE_{int}) and binding energy ($\Delta E_{binding}$). Theoretical calculations show that B compounds are better as corrosion inhibitors than A, C, and D. The addition of NH_2 (B1), NO_2 (B2), CH_3 (B3) substituent in B compounds. By the value of E_{HOMO} , energy gap (ΔE), ionization potential (I), hardness (η), softness (σ) and transferred electrons (ΔN), indicating that the B3 compound have good corrosion inhibition capability.

Keywords: DFT, Corrosion Inhibition, E_{HOMO} , E_{LUMO} .