STUDI TERMODINAMIKA AKTIVITAS ANTIOKSIDAN, TOKSISITAS DAN FARMAKOKINETIKA MOLEKUL SENYAWA FENOLIK EKSTRAK DAUN MATOA (*Pometia pinnata*)

SKRIPSI SARJANA KIMIA

Oleh:

NOVY CRISTHINA NABABAN

NIM : 2110411032

Dosen Pembimbing I : Dr. Imelda, M.Si.

Dosen Pembimbing II : Prof. Dr. Suryati, M.Si.

PROGRAM SARJANA

DEPARTEMEN KIMIA

FAKULTAS MATEMATIKA DAN ILMU PENGETAHUAN ALAM

UNIVERSITAS ANDALAS

PADANG

2025

ABSTRACT

THERMODYNAMIC STUDY OF ANTIOXIDANT ACTIVITY, TOXICITY, AND PHARMACOKINETICS OF PHENOLIC COMPOUNDS IN MATOA (*Pometia pinnata*)

By :
Novy Cristhina Nababan (2110411032)
Dr. Imelda, M.Si.*, Prof. Dr. Suryati, M.Si
***Supervisor**

Matoa (*Pometia pinnata*) is a plant rich in secondary metabolites such as flavonoids and phenolics. These compounds have important biological activities, especially as antioxidants that can neutralize free radicals that cause various degenerative diseases. This study was conducted to theoretically examine the potential of the main phenolic compounds in matoa leaf extract, namely epigallocatechin, apigenin, vanillin, and vanillic acid in antioxidant activity, toxicity, pharmacokinetics, and drug parameters through a computational chemistry approach in the gas phase and water solvents and ethyl acetate. The method used includes molecular structure optimization using Density Functional Theory (DFT) with the B3LYP/6-31G basis set through Gaussian 16W software. Analysis was carried out on thermodynamic properties including the calculation of global reactivity parameters, radical inhibition mechanisms (HAT, SET-PT, and SPLET), pKa values, and toxicity and pharmacokinetic profiles using Marvin Sketch and OSIRIS Property Explorer software. The results showed that all compounds have significant antioxidant activity with different characteristics. Apigenin is the most reactive compound with the lowest bandgap value of 4.0828 eV and the highest dipole moment of 7.0248 Debye. This compound also has the highest electrophilicity of 4.1797 eV indicating a high tendency to capture free radicals. Epigallocatechin has the lowest BDE value at the C5' position of 1612.916 kJ/mol indicating higher efficiency in the HAT mechanism through the release of hydrogen atoms. All molecules release H radicals more easily in water and ethyl acetate solvents than in the gas phase. Analysis of the pKa values shows variations between compounds and the position of the hydroxyl group. Vanillin and apigenin have pKa values close to physiological pH, namely 7.81 (C4) and 7.28 (C5), respectively, which support the ability to ionize under physiological conditions. Pharmacokinetic evaluation shows that all four compounds fulfill Lipinski's Rule of Five. Epigallocatechin has the safest toxicity profile with no mutagenic, tumorigenic, irritation, or reproductive risks. Vanillin, vanillic acid, and apigenin exhibited varying levels of toxicity risk, but still had positive drug scores. The results of this study confirm that phenolic compounds from matoa leaves have strong potential as natural antioxidants and as novel drug candidates, with apigenin and epigallocatechin being the most promising compounds based on their reactivity and safety.

Keywords: *Pometia pinnata*, antioxidant, DFT, toxicity, pharmacokinetics, phenolics