## *ABSTRACT*

## *STUDY OF ESSENTIAL OIL EXTRACTION FROM ROBUSTA COFFEE FLOWERS (Coffea canephora) WITH ORGANIC SOLVENTS AS AROMATHERAPY BY IN SILICO*

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*Robusta coffee flowers (Coffea canephora) are aromatic plant materials known to contain volatile compounds that contribute to their distinctive floral aroma. This study aims to analyze the characteristics of Robusta coffee flower essential oil at different physiological stages and solvent types, including extraction yields, sensory characteristics, chemical composition, and aromatherapy potential through an in silico approach. The research used a Randomized Complete Block Design with two factors, named flower physiological stage (before and after pollination) and solvent types (96% ethanol, acetone, ethyl acetate, n-hexane, and chloroform), with three replications. Extraction was performed using maceration for 24 hours at room temperature followed by solvent evaporation. The results showed that flowers harvested before pollination and extracted using n-hexane produced 0,72% yield and the most distinctive floral aroma. GC-MS analysis indicated that the essential oil was dominated by monoterpenes alcohols, ketones, hydrocarbones, aldehide, and esters. Molecular docking analysis used AutoDock Vina showed that 2,6-octadien-1-ol, 3,7-dimethyl-(Z) exhibited a binding affinity of −6.0 kcal/mol, which was stronger than that of the control ligands linalyl acetate (−5.8 kcal/mol) and borneol (−5.7 kcal/mol). The compound formed aromatic interactions with VAL76 and PHE72, also hydrophobic interactions with LYS235, ILE126, ALA236, VAL224, and VAL227 within the OR1A1 binding pocket, and indicated stable ligand–receptor interactions and had the potential to stimulate the central nervous system associated to the perception of floral aroma that calmed the mind.*



***Keywords:*** *aromatherapy, robusta coffee flower, essential oil, molecular docking*

# ABSTRAK

## KAJIAN EKSTRAKSI MINYAK ESENSIAL BUNGA KOPI ROBUSTA (*Coffea canephora*) DENGAN PELARUT ORGANIK SEBAGAI AROMATERAPI SECARA *IN SILICO*

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Bunga kopi robusta (*Coffea canephora*) merupakan bagian tanaman kopi yang memiliki aroma floral khas karena mengandung berbagai senyawa volatil. Penelitian ini bertujuan mengkaji karakteristik minyak esensial bunga kopi robusta pada perbedaan tahap fisiologis bunga dan jenis pelarut, meliputi rendemen ekstraksi, karakteristik sensori, komposisi kimia, serta potensi aromaterapi melalui pendekatan *in silico*. Penelitian menggunakan Rancangan Acak Kelompok Lengkap (RAKL) dua faktorial, yaitu tahap fisiologis bunga (sebelum dan sesudah penyerbukan) dan jenis pelarut (alkohol 96%, aseton, etil asetat, n-heksan, dan kloroform) dengan tiga ulangan. Proses ekstraksi dilakukan menggunakan metode maserasi selama 24 jam pada suhu ruang dan dilanjutkan dengan evaporasi pelarut. Hasil penelitian menunjukkan bahwa bunga sebelum penyerbukan yang diekstraksi menggunakan pelarut n-heksan menghasilkan rendemen 0,72% dan aroma floral paling khas. Analisis GC-MS menunjukkan bahwa minyak esensial bunga kopi didominasi oleh golongan senyawa monoterpen alkohol, keton, hidrokarbon, aldehid, dan ester. Analisis *molecular docking* menggunakan AutoDock Vina menunjukkan bahwa senyawa 2,6-octadien-1-ol, 3,7-dimethyl-(Z) memiliki nilai *binding affinity* sebesar −6,0 kcal/mol, lebih kuat dibandingkan ligan kontrol linalyl acetate (−5,8 kcal/mol) dan borneol (−5,7 kcal/mol). Senyawa tersebut membentuk interaksi ikatan aromatik dengan VAL76 dan PHE72 serta ikatan hidrofobik dengan LYS235, ILE126, ALA236, VAL224, dan VAL227 pada kantong ikatan OR1A1 dan menunjukkan interaksi ligan–reseptor yang stabil dan berpotensi memicu saraf pusat terkait persepsi aroma floral yang bersifat menenangkan.

**Kata kunci:** aromaterapi, bunga kopi robusta, minyak esensial, *molecular docking*