ABSTRACT

KAJIAN PENYULINGAN MINYAK ESENSIAL BUNGA KOPI ROBUSTA LAMPUNG SEBAGAI AROMATERAPI MELALUI PENDEKATAN *IN SILICO*

BY

MALYA ARIE AMANDA

The utilization of coffee flowers as a source of essential oil remains suboptimal, despite their content of volatile compounds with potential for aromatherapy. This study aims to examine the effect of distillation time on the characteristics of Robusta coffee flower *(Coffea canephora*) essential oil from Lampung and to evaluate its potential for aromatherapy through an in silico approach. Extraction was performed using water and steam distillation methods with varying durations of 0.5–3.5 hours. The study employed a descriptive method with three replicates in the testing process. Testing in the study consisted of yield, sensory characteristics (color and aroma), volatile compound composition via GC-MS, and molecular interaction analysis with the olfactory receptor OR1A1. The results showed that yield increased with longer distillation times, with the best sensory characteristics obtained from pre-pollinated flowers distilled for 2 hours, yielding 0.76%, a color score of 3.7 (light yellow), and an aroma score of 4.9 (very floral). The best treatment (2 hours) indicated that the essential oil of Robusta coffee flowers is dominated by 17 volatile compounds such as benzyl alcohol, trans-linalool oxide, phenylethyl alcohol, benzyl nitrile, 2H-pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-, benzene, (isocyanomethyl)-, 2,6-octadien-1-ol, 3,7-dimethyl-, (z)- , geraniol, 1-tetradecene, benzyl benzoate, 1-tricosene, cetene, 3-octadecene, (e)-, 1-docosene, 1-hexacosene, dan 1-tetracosene. The molecular docking results show that benzyl benzoate, as the dominant compound, has a binding affinity of -7.7 kcal/mol, which is higher than that of the control; it forms an aromatic bond with the TYR265 residue, a hydrogen bond with the LYS186 residue, and hydrophobic interactions with the ALA175, PRO183, and LEU187 residues.

Keywords : essential oil, Robusta coffee flowers, distillation, GC-MS, in silico, aromatherapy

ABSTRAK

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OLEH

MALYA ARIE AMANDA

Pemanfaatan bunga kopi sebagai sumber minyak esensial belum optimal, meskipun kaya senyawa volatile yang berpotensi sebagai aromaterapi. Penelitian ini bertujuan mengkaji pengaruh lama penyulingan terhadap karakteristik minyak esensial bunga kopi robusta (*Coffea canephora*) asal Lampung serta potensinya sebagai aromaterapi secara *in silico*. Ekstraksi dilakukan menggunakan metode penyulingan air dan uap dengan waktu 0,5–3,5 jam. Penelitian dilakukan dengan metode deskriptif 3 kali ulangan. Pangujian dalam penelitian terdiri dari rendemen, karakteristik sensori (warna dan aroma), komposisi senyawa volatil dengan GC-MS, serta analisis interaksi molekuler terhadap reseptor olfaktori OR1A1. Hasil penelitian menunjukkan rendemen meningkat seiring bertambahnya waktu penyulingan, dengan karakteristik sensori terbaik diperoleh pada bunga sebelum penyerbukan dengan lama penyulingan 2 jam, menghasilkan rendemen 0,76%, skor warna 3,7 (bening kekuningan), dan skor aroma 4,9 (sangat floral). Perlakuan terbaik (2 jam), menunjukkan bahwa minyak esensial bunga kopi robusta didominasi oleh 17 senyawa volatil seperti benzyl alcohol, trans-linalool oxide, phenylethyl alcohol, benzyl nitrile, 2H-pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-, benzene, (isocyanomethyl)-, 2,6-octadien-1-ol, 3,7-dimethyl-, (z)- , geraniol, 1-tetradecene, benzyl benzoate, 1-tricosene, cetene, 3-octadecene, (e)-, 1-docosene, 1-hexacosene, dan 1-tetracosene. Hasil molecular docking menunjukkan benzyl benzoate sebagai senyawa dominan memiliki binding affinity sebesar -7,7 kcal/mol, lebih tinggi dibandingkan kontrol, memiliki ikatan aromatik dengan residu TYR265, ikatan hidrogen dengan residu LYS186 dan terdapat interaksi hidrofobik dengan residu ALA175, PRO183, dan LEU187.

Kata kunci : minyak esensial, bunga kopi robusta, penyulingan, GC-MS*, in silico*, aromaterapi