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Solvent Role in Molecular Recognition of Patchouli Extraction Process

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Patchouli or *Pogostemon cablin Benth* is an aromatic plant of importance to the fragrant and cosmetic industries. Its secondary metabolites present interesting pharmacological benefits such as antioxidant and antimutagenic properties. This work is an extended study of the published work in ethanol and water solvents using Ewald summation method and mass spectra characterization of patchouli essential oil extracted with three different polar and non-polar solvents. Ewald summation method has reproduced a better radical distribution function (rdf) intensity in the polar ethanol and water solvents using COMPASS force-field. This work concludes that the complex molecular interaction particularly hydrogen bonding play a significant role to affect the solubility of patchoulol solute either in polar or non-polar solvents during the extraction process.

Keywords: *Pogostemon cablin Benth*, Ewald, Hydrogen bonding.

INTRODUCTION

In medical applications, patchouli essential oil has been reported [1] to inhibit neurogenic pain and also prevents nausea and vomiting [2]. This study aims to recognize the role of the different solvent types in the extraction process of patchouli leaves through molecular dynamics simulation and further correlate infrared and mass spectral data from laboratory experiments.

Ethanol solvent demonstrated a higher content of patchulol marker compound due to the establishment of hydrogen bonding which increased the patchulol solute solubility in the solvent through the OH group [3]. Infrared spectroscopy is able to measure the "free" and "associated" OH-stretch bands and through changes in the relative intensities of the absorption bands, changes in the equilibrium between the free and associated species due to temperature and concentration are attributed [4]. In this work, the hydrogen bonding region in their spectra is of interest as it reflects the solubility of the marker and main solute extracted from the patchouli. Meanwhile, gas chromatography mass spectroscopy (GCMS) is able to identify and provide quantitative and qualitative information on the composition and chemical structures of each compound [5] in the patchouli oil. It combines the power of high resolution separation of components with selective and sensitive mass detection [6].

EXPERIMENTAL

The solvent extraction method is used to extract the patchouli essential oil from samples supplied by Syarikat Nilam Suling Sdn Bhd, Miri, Sarawak, Malaysia. Acetone, ethanol and *n*-hexane were used as the solvents were supplied by Merck (99.7 % purity). Patchoulol leaves (10 g) were macerated in solvent (100 mL) and left overnight. Separation was affected with Buchi Evaporator (R100) and the experiment was replicated three times for each solvent.

The Agilent 7890A Network Sytem gas chromatography equipped with an Agilent 5975C mass spectrometer was used to characterize the extracted oil [3]. Patchoulol (0.02 g) was taken up in 10 mL of each solvent. Then the sample was analyzed using a Perkin Elmer ATR-FTIR spectrometer (Frontier) with spectra range of 4000-500 cm^{-1}. A total 16-32 scans were acquired at 0.15 s/scan and spectral resolution of 2-4 cm^{-1}. The time step of spectral measurement was 2.4-19.2 s/spectrum. The spectra was then analyzed using OMNIC software.

Molecular dynamics simulation: The simulations were carried out in Acceryls Materials Studio (MS), version 5.5, using a HP Z400 workstation. Each solute and solvent molecules geometry was optimized prior to the creation of the simulation boxes. In this study, the condensed-phase optimized molecular potentials for atomistic simulation studies [COMPASS] force field [7] was used to model the system and Ewald summation