UNIVERSITI TEKNOLOGI MARA

ANN MODELLING OF AGARWOOD OIL SIGNIFICANT CHEMICAL COMPOUNDS FOR QUALITY DISCRIMINATION

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AUTHOR'S DECLARATION

I declare that the work in the thesis was carried out in accordancewith the regulations of Universiti Teknologi MARA. It is original and is the result of my own work, unless otherwise indicated or acknowledged as referenced work. This thesis has not been submitted to any other academic institution or non-academic institution for any degree or qualification.

I, hereby, acknowledge that I have been supplied with the Academic Rules and Regulations for Post Graduate, Universiti Teknologi MARA, regulating the conduct of my study and research.

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ABSTRACT

This thesis presents a new ANN modelling in discriminating agarwood oil quality using selected significant chemical compounds of the oil. In order to accomplish the work, the analyses have been carried out in two categories. The first category is the abundances pattern of odor chemical compounds observation and investigation. The extraction of odor chemical compounds is done by solid phase micro-extraction (SPME). In this work two types of SPME fibers were used; divinylbenzene-carboxen-polydimethylsiloxane(DVB-CAR-PDMS) and polydimethylsiloxane(PDMS) to analyze the odor compounds under three different sampling temperature conditions; 40°C, 60°C and 80°C. A consistent abundances pattern of five significant odor chemical compounds as highlighted by Z-score were revealed. The compounds are 10-epi-ϒ-eudesmol, aromadendrane,β-agarofuran, α-agarofuran and ϒ-eudesmol. These odor chemical compounds are important as they contributed to the odor of high quality agarwood oils. Then the second category was performed by the extraction of the agarwood oil chemical compounds using gas chromatography-mass spectrometry (GC-MS). The identified compounds from SPME were used as marker compounds for agarwood oil quality discrimination using GC-MS data. In this category, Z-score highlightedseven significant chemical compounds;β-agarofuran, α-agarofuran, 10-epi-ϒ-eudesmol, ϒ-eudesmol, longifolol, hexadecanol and eudesmol. Their abundances has been used as input to k-nearest neighbor (k-NN) and artificial neural network (ANN) applications. In this study, all the agarwood oil samples were obtained from two institution; Forest Research Institute Malaysia (FRIM) and Universiti Malaysia Pahang (UMP). The experiments were carried out using k-NN and ANN modeling. The study showed that the k-NN classification accuracy is within 81-86% for k=1 to k=5 and 100% accuracy for the classification of ANN modeling.

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CHAPTER ONE
INTRODUCTION

1.1 BACKGROUND

Agarwood oil is the oil extracted from agarwood trees. Agarwood or *gaharu* is the resin impregnated heartwoodof the *Aquilaria* species, a genus which belongs taxonomically to the *Thymelaeaceae* family. The agarwood oil is highly demanded due to its special usage; an incense for religious ceremony, in perfume and traditional medicine preparations [1]. In the Middle East, it is a symbol of wealth and widely used during the wedding ceremony [2-7].

The agarwood oil is traded according to its quality. High quality oil is expensive and low quality is cheap. The oil class also traded basedon its physical properties; color and odor. Usually, dark color and long lasting odor are classified as high quality and sold at premier price [8]. It is normal for a high quality oils to cost between USD126 to USD633 per tola (12ml) [2]. The wood prices for low qualities are USD19 per kg and up to USD100,000 per kg for superior quality [1, 9].

Many studies have been carried out to analyze the quality of agarwood oil [10-14]. Researchers from Japan has classified Kanankoh as the highest quality among many types of agarwood oil and Jinkoh as the low quality [11, 13, 14]. The relationship between high and low quality of oil has been widely investigated by comparing their chemical compositions [13, 14]. One of the investigations found that the abundances (percentage relative peak area measured by GC-MS) of the same compound in high quality oil is more than in low quality [14].

There are many techniques available to analyse the chemical compounds of essential oils; electronic nose (Enose), gas chromatography (GC), gas chromatography/mass spectrometric (GC-MS), solid phase micro extraction (SPME), gas chromatography –flame ionization detector (GC-FID), gas chromatography-olfactometry (GC-O) and comprehensive two dimensional gas chromatography (GCxGC) [12, 14-19].GC-O is the odor-compounds extraction method with combining gas chromatography and human sensory panel [19]. This method is limited to the subject of fairness since human nose cannot tolerate with many samples at the same time [15]. In GC x GC, chemical compounds are separated by a single column