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ANN Modelling of Agarwood Oil Significant Chemical Compounds for Quality Discrimination

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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- γ -eudesmol, aromadendrane, β -agarofuran, α -agarofuran and γ -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 highlighted seven significant chemical compounds; β -agarofuran, α -agarofuran, 10-epi- γ -eudesmol, γ -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.