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THE STUDY OF PHYSICOCHEMICAL PROPERTIES OF THYMOL-BASED HYDROPHOBIC DEEP EUTECTIC SOLVENTS

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THE STUDY OF PHYSICOCHEMICAL PROPERTIES OF THYMOL-BASED HYDROPHOBIC DEEP EUTECTIC SOLVENTS

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This Final Year Project Report entitled **"The Study of Physicochemical Properties of Thymol-Based Hydrophobic Deep Eutectic Solvents"** was submitted by Aesyah Sofea Khairurrushdi Binti Roslan in partial fulfilment of the requirements for the Degree of Bachelor of Science (Hons.) Applied Chemistry, in the Faculty of Applied Sciences, and was approved by

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ABSTRACT

THE STUDY OF THYMOL-BASED HYDROPHOBIC DEEP EUTECTIC SOLVENTS

An increase in popularity of non-toxic products in place of conventional hazardous organic solvents has led to a focus on the development of environmentally friendly hydrophobic deep eutectic solvents (HDES). This research presented the development and evaluation of several thymol-based HDESs using three fatty acids (hexanoic, nonanoic and decanoic) as hydrogen bond acceptors (HBAs). FTIR spectroscopy demonstrated the formation of a deep eutectic through significant changes to the OH stretching vibrations (3198 cm^{-1} to ~2919-2964 cm^{-1}) and C=O bands, indicating there is a strong intermolecular hydrogen bond. The data also indicates the molar ratios and chain length of fatty acid alkyl chains have a significant impact on the physicochemical properties of the HDESs. In addition, thermal analysis indicated the standard protocol of holding at 40ºC was inadequate for achieving equilibrium for certain combinations of Thymol:hexanoic acid (THYHA). So, the analysis showed that higher temperatures and a period of isothermal soaking is required for the achievement of thermal equilibrium. Data indicated THYHA (C6) had the highest density (0.653 g/cm^3) out of all of the HDESs due to the direct correlation between molar ratios of molecules and packing density. The antibacterial activity of all of the HDESs against Gram-positive bacteria having the highest inhibition zone of 18.4 mm for THYHA, and the levels of toxicity resulted from the Brine Shrimp Lethality Assays indicate that the high levels of mortality were likely due to physical asphyxiation from the air/water interface and not due to chemical toxicity. Future work will require more advanced techniques to measure viscosity and conductivity, along with the development of advanced models for determining toxicities of hydrophobic solvents.