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Antibacterial performance enhancement using hydrophobic deep eutectic solvents: COSMO-RS prediction, experimental validation, and synergistic action with antibiotics

(2024) *Journal of Molecular Liquids*, 396, art. no. 124008, . Cited 2 times.

DOI: 10.1016/j.molliq.2024.124008

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Abstract
Microbial infection is a hazardous and challenging clinical problem that has attracted considerable attention recently, primarily owing to the noticeable rise in antimicrobial resistance. To address the medical requirements to encounter this dilemma, we present hydrophobic deep eutectic solvents (HDESs) that combine experimental research and computational prediction; conductor-like screening model for real solvents (COSMO-RS). Menthol-based HDESs were successfully obtained when mixed with fatty acids, and their thermal profiles were analyzed. The HDES systems and their synergistic effects demonstrated potent antimicrobial activity against Gram-positive and Gram-negative bacteria, with DES 4 (menthol:decanoic acid) exhibiting the highest bactericidal activity at a molar ratio of 1:5. The interaction between the HDESs and bacterial cell wall structural compounds was confirmed by field-emission scanning electron microscopy and Fourier transform infrared spectroscopy. The results revealed a favorable concurrence between the projected and empirical outcomes, indicating that DES 4 exhibited bacteriostatic properties and could be a viable substitute for managing bacterial infections of diverse origins. In addition, the synergistic effect of DES 4 and tetracycline showed promising potential. The successful integration of experimental and computational approaches in this study also sets a precedent for the rational design of future antimicrobial agents and opens new avenues for tackling other clinical challenges. © 2024 Elsevier B.V.

Author Keywords
Antimicrobial resistance; Bacterial infection; Green antibacterial agent; Hydrophobic deep eutectic solvents; Ionic liquid; Synergistic effect

Index Keywords
Alcohols, Antimicrobial agents, Bacteria, Cell membranes, Diagnosis, Eutectics, Field emission microscopes, Fourier transform infrared spectroscopy, Hydrophobicity, Ionic liquids, Molar ratio, Scanning electron microscopy, Solvents; Antibacterial performance, Antimicrobial resistances, Bacterial infections, Conductor-like screening model for real solvents, Deep eutectic solvents, Green antibacterial agent, Hydrophobic deep eutectic solvent, Hydrophobics, Performance enhancements, Synergistic effect; Fatty acids

Funding details
Ministry of Higher Education, MalaysiaMOHE

The authors express their gratitude to the Ministry of Higher Education in Malaysia for generously providing the grant to support this research. The authors sincerely appreciate the high-quality FESEM analysis provided by Mr. Mohd Shukri Aziz (Senior Assistant Science Officer), from the Chemistry Department, Faculty of Science, Universiti Malaya.

The authors express their gratitude to the Ministry of Higher Education in Malaysia for generously providing the grant to support this research. The authors sincerely appreciate the high-quality FESEM analysis provided by Mr. Mohd Shukri Aziz (Senior Assistant Science Officer), from the Chemistry Department, Faculty of Science, Universiti Malaya.

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Publisher: Elsevier B.V.

ISSN: 01677322
CODEN: JMLID
Language of Original Document: English
Abbreviated Source Title: J Mol Liq
2-s2.0-85182906374
Document Type: Article
Publication Stage: Final
Source: Scopus