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COSMO-RS Based Prediction and Screening of Antimicrobial Activities of Deep Eutectic Solvents
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Abstract

A total of 18 different deep eutectic solvents (DESs) were thoroughly analyzed in this extensive study employing the most recent advances in COSMO-RS (Conductor-like Screening Model for Real Solvents) analytical approach. To establish a broad and representative sample for the study, these DESs were carefully chosen and made up of a range of substances, including urea, thymol, menthol, and six different fatty acids. This study's main goal was to examine the various DESs' antibacterial capabilities by examining how they interacted with bacterial cells. The study concentrated on looking at how the DESs interacted with four crucial bacterial cell components in order to accomplish this aim. Components were 2,6-diaminopimelic acid, N-acetyl- α -neuraminic acid, N-acetyl-muramic acid, and N-acetyl-D-glucosamine. These elements were chosen because they play important roles in the construction and operation of bacterial cells. The results of the research showed that the advanced σ -profiling and σ -potential assessments offered useful information on the most interactive and successful DESs against microbial cells. Decanoic acid-based solvents showed the most effectiveness in interacting with the chosen bacterial cell components among the 18 DESs tested. This study's significance and effects go beyond its immediate conclusions. In order to save resources in creating new antimicrobial drugs, this study provides a simplified method for screening biological components. Furthermore, this research opens doors for further investigation and potential applications of these solvents in the fight against drug-resistant bacteria and the development of new therapeutic approaches for treating infectious diseases by identifying Decanoic acid-based DESs as potent antimicrobial candidates. © The Author(s), under exclusive license to Springer Nature Switzerland AG 2024.

Author Keywords

Active pharmaceutical ingredients; Antimicrobial activity; COSMO-RS; Deep eutectic solvents

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