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Theoretical and experimental evidence for the use of natural deep eutectic solvents to increase the solubility and extractability of curcumin

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ABSTRACT

Natural Deep Eutectic Solvents (NADESs) are a novel class of environmentally friendly liquids that can replace traditional organic solvents in industrial applications due to their ecologically beneficial features. These novel organic solvents are formed via weak interactions (mostly H-bonds) between two or more naturally existing substances. Even though they were recently found and recognized, NADESs have been the subject of significant and exciting research due to their unique properties. This study aims to determine the thermodynamic properties of eight NADESs and their solubility towards curcumin, a naturally occurring substance with significant medicinal properties. This study used a dual in-vitro and in-silico strategy: first, NADESs were characterized using Fourier transform infrared spectroscopy; second, various combinations and mixes were simulated using the Turbomole and COSMOThermX tools. Additionally, it was discovered that the curcumin activity coefficient in the NADES1 is −0.31 higher than that of the other NADESs (0.23–3.4) or the individual components (2.4–5.4) and water 8.9. The findings demonstrated that the studied NADESs had critical structural features in H-bonding and curcumin solubilization capabilities.

1. Introduction

Due to their unique features, including biodegradability, inflammability, nontoxicity, and low melting temperatures, Deep Eutectic Solvents (DESs) have emerged as viable alternatives to regularly used organic liquids. Additionally, although DESs have many properties with ionic liquids (ILs), they offer several benefits over ILs, including ease of preparation, low cost, and biodegradability [1]. DESs may be made by heating two or more components to a reasonable temperature and mixing them [2]. DESs have been evaluated for a variety of applications, including CO2 capture [3], nanotechnology [4], gas purification [5], extraction [6], and various other chemical and industrial processes. Choi et al. [7] have recently discovered a relevant class of DESs known as natural deep eutectic solvents (NADESs). It has been shown that when specific molar ratios of primary metabolites from plants, such as sugars, choline, and amino acids, were mixed at moderate temperature, they may form a DES. The preparation of NADES is similar to that of DESs in that it involves combining an HBA (Hydrogen Bond Acceptor) and an HBD (Hydrogen Bond Donor) in a particular molar ratio, stirring, and heating until a homogenous liquid is formed without the use of any other solvent [8]. NADESs components are characterized by various functional groups such as carboxylic acids, carbonyl, and hydroxyl, creating an intermolecular

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