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Prediction of solvatochromic parameters of eutectic solvents to extract macroalgae sterols using COSMO-RS

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PURPOSE OF THE ABSTRACT

Macroalgae are considered a promising source of a wide range of added-value secondary metabolites. Sterols, in particular, have caught attention due to their antibacterial, anti-inflammatory, and antiproliferative activities, which may be exploited in pharmaceutical or nutraceutical applications [1]. However, the conventional methods of extraction of these compounds relying on organic (often toxic) solvents, and their high cost and low efficiency, are major drawbacks limiting the use of sterols in such fields. Eutectic Solvents (ES) provide innovative solutions fulfilling the principles of Green Chemistry to reduce or eliminate hazardous substances, and may afford an eco-friendly route for the selective extraction of bioactive components from macroalgae [2].

To deal with the numerous combinations of hydrogen bond acceptors (HBA) and donors (HBD) to form ES, here, the conductor-like screening model for real solvents (COSMO-RS) [3] was used as an initial screening tool to select the most suitable combination from a pool of thirty-five HBA and sixty-four HBD (total of 2240 mixtures). ES comprising fatty acids and terpenes, as HBA/HBD, and some alcohols, as HBD, are found to be the most suitable solvents for sterols extraction. These ES were applied in solid-liquid extractions of Codium tomentosum and the ability to obtain an extract rich in sterols was evaluated and compared with conventional extractions.

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FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

Eutectic solvents | Macroalgae | Sterols | COSMO-RS

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