Screening of Suitable Ionic Liquids as Green Solvents for Extraction of Eicosapentaenoic Acid (EPA) from Microalgae Biomass Using COSMO-RS Model

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Abstract

Omega-3 poly unsaturated fatty acids (PUFA) particularly eicosapentaenoic acid (EPA), and docosahexaenoic acid (DHA), have many health benefits including reducing the risk of cancer and cardiovascular disease. Recently, the use of ionic liquids (ILs) in lipid extraction from microalgae provides the potential to overcome common drawbacks, offers several other benefits. To date, very limited researches are available to focus on extracting microalgae lipid and PUFA in particular by using ILs. The objective of current work is to screen the potential ILs that can be applied in EPA extraction. In this study, fast ILs screening was performed with the help of a conductor like screening model for real solvents (COSMO-RS) and the ILs with higher capacity values for use in extraction of EPA were compared. According to the results, the highest capacity for EPA extraction among 352 screened cation/anion combinations belongs to [TMAm][SO4]. It is expected to achieve a higher yield of EPA once applying this combination as the solvent in the process of extraction. ILs with small anions were observed to have higher capacities, as well possessing higher charge density compared to larger ones, and therefore, they are more preferable for extraction purposes. Moreover, shorter alkyl chain cations are preferred when using imidazolium-based IL, which agrees with experimental data.

Keywords

Author Keywords: COSMO-RS; omega-3; EPA extraction; ionic liquids; screening; extraction capacity; infinite dilution activity coefficient

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