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## Screening of Ionic liquids for PUFA extraction from microalgal biomass using COSMO-RS

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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, cardiovascular disease, autoimmune, inflammatory disorders, cystic fibrosis, disrupted neurological function, bowel disease and mental illness. The EPA and DHA from microalgae are favorable due to algal is farmed in a controlled environment that avoids harmful contamination such as methyl mercury, copper from the sea. Moreover, microalgae oil do not have the problem to deficiency of vitamin E unlike fish oil. It has also the advantage of presenting neither an unpleasant odour nor a high amount of cholesterol, and contains squalene and phytosterols, which offer additional benefits to human health. However, the existing conventional methods of lipid extraction like soxhlet consume large amount of solvent and consider as high toxic and energy intensive methods. Ionic liquids (ILs) is one of the new classes of solvent that has potential in extracting the microalgae PUFA. It provides low vapor pressure, high thermal stability, non-toxicity and dissolve polar, non polar organic, inorganic and polymeric components. However, very limited research has been conducted on extracting microalgae PUFA using ILs. Therefore, this study aims to screen the potential ILs that can be used in the microalgae extraction process. The screening work was carried out using Continuum Solvation Models for Real Solvents (COSMO-RS). In this research use cosmo-rs to investigate the effect of hydrophilic and hydrophobic anions base ILs and also effect of the increase alkyl chain length from C<sub>2</sub> to C<sub>8</sub> on the EPA and DHA extraction. Cosmo-rs done this simulation by the calculation of activity coefficient ( $\gamma$ ). It was found that the lowest activity coefficient has the best interaction between the solute and solvent. According to the results lowest activity coefficient for EPA and DHA extraction belong to [Cl] as anion for the imidazolium, pyridinium and pyrrolidinium with different alkyl chains. The effectiveness of those combinations will be further tested in the microalgae extraction.

**Keywords:** microalgae, biomass, ionic liquid, PUFA, COSMO-RS