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Abstract. The concept of sustainable and green solvent has always highlighted in the field of energy and environmental science. The synthesis and application of natural-based Low Transition Temperature Mixture (LTTM) as a novel and green solvent for the lignocellulose biomass pre-treatment such as delignification of Oil-Palm Empty Fruit Bunch (EFB) have been greatly emphasized. In this present work, the investigation of LTTM efficiency as green solvent in delignification process was conducted using both theoretical and experimental studies. Initially, screening of solvation properties of different types of hydrogen bond acceptor (HBA) and predicted hydrogen bond donor (HBD) for synthesis of LTTMs was conducted using conductor-like screening model (COSMO-RS) software and formation of hydrogen bonding was evidenced using NMR spectroscopy analysis. Three types of HBA namely sucrose, choline chloride and monosodium glutamate were mixed with malic acids as HBD and their charge density distribution on the surface was determined through sigma profile (σ). The COSMO-RS results determined the σ profile of pure component malic acid to be 11.42, sucrose to be 25.37 and the total value of σ profile for mixtures is 14.19 as the best combination of LTTM composition compared to LTTM from choline chloride and monosodium glutamate (MSG). The reliability of the COSMO-RS predictions data was correlated with Nuclear Magnetic Resonance (NMR) analysis through determination of peaks with chemical shifts hydrogen bonding that suggested existence of potential interaction between malic acids and sucrose has occurred.

1. Introduction

The dependency of fossil fuels leads to the environment problems such as environmental contamination and global heating. Thus, most researchers are looking for bio-based materials that can offer renewable, biodegradable, and biocompatible sources as alternative to fossil based materials. According to researchers Ong & Wu [1] Zhang *et al.* [2], Zakzeski *et al.* [3] and others, lignocellulosic biomass as