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Automated Fast Computational Screening of Solvents for Extraction of Organic Chemicals from Aqueous Solution Using SMD Solvation Free Energies

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Abstract: Extraction of organic chemicals is a usual problem in chemistry. However, identification of the best solvent for extraction is not obvious and is usually based on try and error approach. With the development of continuum solvation models like SMD, which is parametrized for a wide set of solvents, it is possible to make a screening of different solvents for extraction. In this work, this idea was applied for finding the best solvent for extraction of chemicals derived from biomass decomposition. Biomass is one of the most promising alternatives for petroleum substitution due to its abundance, low cost and environmentally harmless. Three potential compounds from biomass were listed for fuel and chemical production: furfural, 5-hydroxymethylfurfural and levulinic acid. The acid catalyzed hydrolysis of xylan and glycan components of the wood form C_5 and C_6 sugars, so xylose and glucose (or fructose) are transformed into furfural, 5-hydroxymethylfurfural (HMF) and levulinic acid via acid-catalyzed dehydration. Nevertheless, in the acid medium, undesirable products may appear during the process. Thus, the use of solvent extraction has been advocated as a more effective process. In this work, we are looking for an adequate solvent, which should have low miscibility with water and lead to a high partition coefficient for each compound. We used the SMD method, which has parameters for 179 solvents. We have written the "SNAPY", a code in Python programming language to automate the process of building the input files, running the GAMESS program and reading the solvation free energy values from the output. In the selection of solvents for simultaneous extraction of furfural, HMF and levulinic acid, we have done an analysis to suggest solvents with the highest partition coefficients (aqueous/organic solvent) for all the solutes. In addition, the solvents must have low miscibility with water, boiling point below 162 °C (furfural boiling point) and, preferentially, low toxicity. Thus, the manual analysis of the results has led us to suggest that C_6 and C_7 ketones are the most adequate solvents.[1]

Key-words: partition coefficient, green chemistry, solvation model, free energy of transfer

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References:

[1] Dalessandro, E. V.; Pliego Jr. J. R., *Fast Screening of Solvents for Simultaneous Extraction of Furfural, 5-Hydroxymethylfurfural and Levulinic acid from Aqueous Solution Using SMD Solvation Free Energies. J. Brazil. Chem. Soc.* **2017,** (in press)