

## Choline chloride-based deep eutectic solvents: A computational and experimental study for extraction of flavonoids and phenolic compounds from soybean and okara

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This study aimed to use COSMO-SAC software to screen a set of solvents by evaluating the activity coefficient at infinite dilution of the isoflavones daidzein, genistein, glycitein, daidzin, genistin, and glycitin followed by experimental validation. COSMO-SAC screening was performed with 18 solvents, thirteen deep eutectic solvents (DES) containing choline chloride (ChCl) as HBA, and different carboxylic acids, sugars, and polyols as HBD. In addition to DES, water, 70% ethanol, 80% methanol, 70% ChCl, and 70% acetic acid were evaluated. With the best solvents, extraction experiments were performed for validation. Initially, soybean and okara were weighed and mixed with the solvents in test tubes of 10 mL (solid-solvent ratio 20 mg/mL). The tube was placed inside 50 mL containers containing water and jacketed for circulating water from a thermostatic bath to maintain the temperature. Extractions were performed by heating the mixture to 60 °C, under constant magnetic stirring at 600 rpm for 60 min. After the extractions, determinations of total flavonoids were carried out. After computer screening, it was found that the solvents with the highest interaction with the analytes were: 70% ethanol, 80% methanol, 70% acetic acid, 70% ChCl, and the DES ChCl: acetic acid, ChCl: lactic acid, ChCl: glycerol, ChCl: formic acid. The DES ChCl: glucose presented the worst performance in the computational modeling and was also used for validation. Experimentally, the solvents that most extracted isoflavones from soybean were ChCl:acetic acid>70% Ethanol>70% acetic acid>80% Methanol>70%ChCl>ChCl:lactic acid>ChCl:glycerol>ChCl:formic acid>ChCl: glucose. For okara, the best solvents were ChCl:acetic acid>Methanol 80%>ChCl 70%>ChCl:lactic acid>acetic acid 70%>Ethanol 70%>ChCl:formic acid>ChCl:glycerol>ChCl:glucose. Furthermore, it was observed that all total flavonoid results were higher for soybean, with the maximum concentration of 1.05 mg equivalent of catechin/g of the sample obtained with DES ChCl: acetic acid. Therefore, COSMO-SAC can be used as a tool to assist in the screening of solvents in extraction processes and DES can be used as an alternative for the extraction of isoflavones, replacing conventional solvents such as ethanol and methanol.