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Influence of DES on the formation of organic biphasic systems for separation of natural compounds.

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PURPOSE OF THE ABSTRACT

In the current context of sustainable development and circular economy, new sustainable processes and techniques for obtaining pure natural compounds is subject of intense studies. Recent works [1,2] have reported that Deep Eutectic Solvents (DES) added to two miscible organic solvents (e.g., ethanol and heptane) trigger a phase demixion and the formation of a biphasic system, that can be further applied to the partitioning of natural compounds.

In order to get a better understanding at the mechanisms in play for the formation of biphasic systems, twelve biphasic systems containing heptane, either ethanol, 1-butanol, or ethyl acetate (EtOAc), and either hydrogen bond donor compounds (HBD), glycerol, ethylene glycol (EG), levulinic acid (LevA), or the corresponding choline chloride-based DES were studied as potential extracting systems for six natural compounds, namely, quercetin, apigenin, coumarin, beta-ionone, retinol, and alpha-tocopherol. Phase diagrams for all biphasic systems were measured using cloud-point titration. Phases compositions were measured using GC-FID and HPLC. Partitions coefficients of the natural compounds were evaluated using HPLC. Binodal curves and partition coefficients were also predicted using a conductor-like screening model for real solvents (COSMO-RS). Calculated and experimental results are in good agreement, confirming that COSMO-RS is a useful and promising tool for screening such complex biphasic systems to find the most adequate system for purifying specific natural compounds. For systems containing ethanol it appears that the polarity of the HBD is the most relevant property driving the phase separation and that choline chloride has only a minor influence on the phase diagram and on the partition of the natural compounds [3]. On the contrary, in systems containing ethyl acetate or 1-butanol, choline chloride has an increased influence on the phase separation reducing the amount of 1-butanol or ethyl acetate in the lower phase. This, in turn, also affects the partition coefficient of a natural compound. When the latter is present in both phases, addition of choline chloride mostly moves a natural compound towards the upper phase. Presence of choline chloride thus becomes critical when ethanol is substituted with ethyl acetate or 1-butanol. This opens new possibilities for modifying such biphasic systems for separation of natural compounds, for example using centrifugal partition chromatography (CPC).

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FIGURES

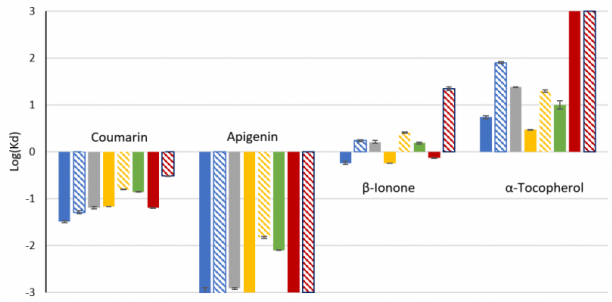

FIGURE 1

Partition coefficient (log(Kd)) of the natural compounds in different biphasic systems.
Blue: Heptane-Ethanol-LevA; Hatched blue: Heptane-Ethanol-ChCl:LevA; Grey: Heptane-Ethanol-EG; Yellow: Heptane-1-Butanol-LevA; Hatched yellow: Yellow: Heptane-1-Butanol-ChCl:LevA; Green: Heptane-1-Butanol-EG; Red: Heptane-EtOAc-LevA; Hatched red: Hept

FIGURE 2

KEYWORDS

Organic biphasic systems | partition coefficients | natural compounds | COSMO-RS

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