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Investigation of Hexafluoroisopropanol-Based Aqueous Biphasic System

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Aqueous biphasic system (ABS) is a liquid-liquid fractionation technique, which has gained an interest because of great potential for the extraction and enrichment of various organic and inorganic pollutants from aqueous samples [1]. ABS formation, which is a kind of soluting-out phenomena, appears when combination of two water miscible compounds display incompatibility in aqueous media above critical concentrations [2, 3]. Typical mixtures are composed of two hydrophilic polymers or salts, or a combination of polymer and salt [4, 5]. However, since volatile organic compounds are not employed in such systems, they are hardly compatible with modern separation techniques such as chromatography with its various modes.

In this study, a novel hexafluoroisopropanol (HFIP) based ABS system was investigated and its extraction properties for the extraction of various organic compounds from aqueous solutions were tested.

In initial experiments, common polar organic solvents (acetonitrile, ethanol, isopropanol, acetone, dimethylsulfoxide, dimethylformamide and tetrahydrofuran) were tested as soluting-out agents of the HFIP phase. The ABS formation procedure was done in the following order: 5.0 mL of 0.02 mmol/L aqueous alizarin solution was placed into a glass centrifuge tube, then 3.0 mmol soluting-out agent and 0.3 mL HFIP were sequentially added. The mixture was shaken manually for 30 s, resulting in the formation of emulsion. The phases were separated by centrifugation at 3000 rpm for 5 min. Alizarin dye was added into the water solution to visualize the phase separation. Obtained results showed that only aprotic solvents act as soluting-out agent. The formed HFIP phase volumes decrease in the following order: tetrahydrofuran > acetone ≈ dimethylformamide > ACN > dimethylsufoxide. This indicates that soluting-out ability of the solvents correlates with their hydrophilicity: higher HFIP phase volumes were obtained using less hydrophilic soluting-out agents.

Next, the extraction properties of the HFIP-ACN-based ABS system were evaluated. Aromatic hydrocarbons, esters, hydroxyesters, amines, carboxylic acids, phenols and synthetic dyes were employed as model analytes. As expected, for structurally related analytes their extraction efficiency values showed good correlation with their hydrophobicity (i.e., log *P* values). For example, the extraction efficiencies of hydroxyesters (parabens) increase in the following order: methylparaben < ethylparaben < propylparaben < butylparaben. Such trend was also observed within other analyte groups studied.

Surprisingly, in contrast to conventional organic solvents, proposed ABS system exhibits significant extraction selectivity within different classes of analytes having close hydrophobicity. For selected analytes with similar log *P* values, their extraction efficiencies decrease from 98% (nicotine) to 25% (benzoic acid) in the following order: nicotine ≈ dimethylphthalate ≈ benzene > methylparaben > quercetin ≈ benzoic acid. This suggests that the ABS system exhibits significantly better extractability for basic and neutral organic compounds comparing with acidic ones.

The obtained results demonstrate that developed HFIP-ACN-based ABS system may be considered as very promising alternative extractant for various organic compounds from aqueous samples.

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