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Original Research Article

Investigations of Hg(II) analysis in real samples via computational chemistry, experimental design, and green microextraction approach

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ABSTRACT

An economical and green nanostructured supramolecular solvent-based ultrasound-assisted homogeneous liquid-liquid microextraction procedure was developed to separate and preconcentrate Hg(II) ions in water and vegetable samples in the presented article. The interactions between chemical species were investigated using computational chemistry. The experimental design was used to optimize critical variables influencing the separation of Hg(II). Under optimum conditions (pH = 6.4; the volume of supramolecular, 170 μL; the amount of ligand, 14 mmol L^{-1}; extraction temperature, 35 °C), the linearity was in the range of 1–450 μg L^{-1}. The procedure has an enrichment factor of 82 with a detection limit of 0.33 μg L^{-1}. In addition, repeatability and reproducibility precisions for 10, 100, and 300 μg L^{-1} of Hg(II) were in the range of 1.8–3.4 % and 2.5–4.4 %, respectively. The accuracy was tested by analyzing certified reference materials and then successfully applied for the pre-concentration and determination of Hg(II) ions in the selected samples with relative recovery.