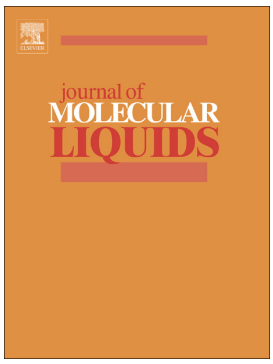

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Liquid phase extraction of nanosized biologically active estrogenic pollutants by using an efficient adsorbent

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Abstract

Dangerous nanosized micropollutants and estrogenic hormones which might severely affect the environment are more found in water effluents, recently, and detection of them is of high importance. As the result, reliable and inexpensive absorptive extraction and removal applications are favored. As the second most abundant biomolecule on earth, a lignocellulosic material can be a potential choice as nanosized adsorbent. In this paper, quantum chemistry techniques are employed as the state of the art approach for predictive modeling, to investigate the feasibility of using this material in extraction and removal of of eight estrogens including estradiol, estrone, testosterone, progesterone, estriol, mestranol, ethinylestradiol and diethylstilbestrol. Due to nano-scaled dimensions of these pollutants, removing them by using current commercial methods is challenging and a new approach needed to be developed. The mechanism of removing micropollutants from water affluent is based on adsorption. This fact motivated us to simulate the adsorption process, and check how well the adsorbent interact with nanosized micropollutants. In order to evaluate the affinity of lowest energy sites on structure of the lignocellulosic material toward each estrogenic hormones and micropollutants, we carried out configurational bias Monte Carlo search of the configurational space of the lignocellulosic material-estrogenic micropollutants systems according to a simulated annealing schedule. To check the response and sensitivity of the lignocellulosic material to each estrogenic micropollutants, a combination of modified Flory-Huggins model and molecular simulation techniques was used. Evaluation of detachment energy revealed the potential of the lignocellulosic material as a reusable material for removing these compounds in an aqueous media.

Keywords: estrogenic micropollutants, water effluent, biosensors, computational chemistry, molecular modeling

1. Introduction

As a consequence of usage of hormonal drugs in disease treatments, various types of biologically active nanosized micropollutants such as estrogens are released into environment,

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