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Adsorption isotherm and kinetic analysis of molecularly imprinted polymer with two functional monomers for quantification of atrazine

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Abstract

The extensive use of atrazine as a pesticide in agricultural practices poses a significant risk to the environment and human health. Atrazine, when applied to plants, has the potential to migrate through the soil and contaminate groundwater sources. Consequently, there is an urgent need to explore alternative methods for detecting atrazine. This study aimed to investigate the quantification of atrazine using molecularly imprinted polymer (MIP) and to assess the adsorption performance and kinetics of the MIPs using various isotherm and kinetic adsorption models. MIP was synthesised with two distinct functional monomers: methacrylic acid (MAA) and acrylamide (AA). Computational analysis was employed to estimate the binding affinity of these monomers towards atrazine. Subsequently, results from adsorption capacity study indicated a higher binding affinity for MAA compared to AA with values of 0.92 mg/g and 0.48 mg/g, respectively. These findings aligned with the simulated data from the docking analysis. Moreover, the adsorption mechanism of atrazine towards MIP-MAA and MIP-AA was best represented by Jovanovic model, followed by the Langmuir, Freundlich and Linear models. While for kinetics analysis, the Elovich model was chosen as the best fit. In conclusion, the selection of the functional monomer is of utmost importance in designing MIPs as it facilitates specific interactions with analyte molecules and enhances the performance of the MIPs. © 2023 Informa UK Limited, trading as Taylor & Francis Group.

Author Keywords

adsorption isotherm; atrazine; binding affinity; functional monomer; Molecularly imprinted polymer

Index Keywords

Adsorption, Adsorption isotherms, Amides, Binding energy, Binding sites, Groundwater, Groundwater pollution, Health risks, Kinetics, Monomers; Acrylamides, Adsorption kinetics, Agricultural practices, Binding affinities, Functional monomer, Groundwater sources, Human health, Kinetic analysis, Methacrylic acids, Molecularly Imprinted Polymer; Herbicides

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