



ADSORPTION AND MOLECULAR DOCKING STUDY OF BISPHENOL A USING REUSABLE ZIF-8 (Zn) METAL-ORGANIC FRAMEWORKS IN AN AQUEOUS SOLUTION

(Penjerapan dan Kajian Penambatan Molekul Bisfenol A Menggunakan Kerangka Logam-
Organik ZIF-8 (Zn) yang boleh Digunakan Semula dalam Larutan Air)

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Abstract

Bisphenol A (BPA) is a derivative of phenol that has been identified as a pollutant in water. This work aimed to evaluate the experimental and molecular docking findings on the adsorption of BPA using porous material metal-organic frameworks (MOFs) of zeolitic imidazolate frameworks (ZIF-8 (Zn)). The commercial ZIF-8 (Zn) was characterized by field emission scanning electron microscopy (FESEM), scanning electron microscopy (SEM), and energy dispersive X-ray (EDX). The surface morphology of ZIF-8 (Zn) showed cubic particles and zinc components (18.70 %) detected by EDX. The adsorption of endocrine-disruptive chemicals of BPA was performed by batch adsorption experiments and measured using ultraviolet-visible (UV-Vis) spectrophotometry. ZIF-8 (Zn) was shown to achieve adsorption at BPA dosage (0.4 g), and pH 6 (25 °C) with high BPA removal (98.84%). Molecular docking simulation represented that BPA was bound to ZIF-8 (Zn) via the inner pores. The mechanism interaction of BPA and ZIF-8 (Zn) was via van der Waals interaction. The adsorption of BPA onto ZIF-8 (Zn) fitted the Langmuir isotherm and the pseudo-second-order model. The possible regeneration and reusability of ZIF-8 (Zn) show good suitability for reusable adsorbent in BPA adsorption application from environmental water.

Keywords: bisphenol A, adsorption, ZIF-8, water pollutants, metal-organic frameworks

Abstrak

Bisfenol A (BPA) adalah terbitan fenol yang telah dikenal pasti sebagai bahan pencemar di dalam air. Kerja kajian ini bertujuan untuk menilai eksperimen dan kajian penambatan molekul pada penjerapan BPA menggunakan kerangka kerja logam-organik (MOFs) bahan berliang iaitu kerangka besi zeolitik imidazolat (ZIF-8 (Zn)). ZIF-8 (Zn) secara komersil dicirikan oleh mikroskopi electron imbasan pancaran medan (FESEM), mikroskopi electron elektron imbasan (SEM), dan sinar-X serakan tenaga (EDX). Morfologi permukaan ZIF-8 (Zn) oleh EDX menunjukkan zarah padu partikel kubik dan komponen zink (18.70 %) dikesan oleh