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Adsorption of Metronidazole Drug in MOF by Monte Carlo Simulation

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Metal-organic frameworks (MOFs) are a new type of nano-porous [1] coordination networks [2] which composed of metal ions or clusters linked by organic ligands [3]. Metal-organic frameworks due to the characteristics of both groups, are considered as suitable materials in drug delivery [4, 5]. Generally, in recent years, MOFs have received much attention which is attributed to their unique surface areas and permanent porosity. MOFs are showed great promise in various applications such as gas storage, gas separation, shape/size selective catalysis, drug storage and delivery, imaging, and sensing [6]. Therefore, grand canonical Monte Carlo (GCMC) simulations were used in this work to investigate the adsorption behavior of metronidazole in MOF-5 as a carrier of drug [7]. A typical GCMC simulation was carried out for 1000000 step, in which the first 200000 step were used for equilibration followed by 800000 steps to sample the desired properties. All the simulations are performed at 36.5 and 37.5 °C and at pressures varying between 0-100 kPa. The results showed that the maximum adsorption of metronidazole in MOF-5 is 43 units per cell at 100 kPa and 37.5 °C. In general, metronidazole adsorption on MOF-5 in the aqueous environment is similar to the adsorption in pure MOF-5 at the all ranges of investigated temperatures and pressures. Also, metronidazole uptake in other metal organic frameworks showed that MOF-177 has the highest drug adsorption than MOF-5. Finally, the results of the present study suggested MOF-5 has a suitable potential as a carrier of metronidazole.

Keywords: *Metal Organic Framework, Metronidazole, Drug Carrier, Simulation*

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