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Synthesis, application and molecular docking of modified cellulose with diaminoguanidine as complexing agent for selective separation of Cu (II), Cd (II) and Hg (II) ions from alum sample

Heba E. Saad^{1,2}, Yusif S. El-Sayed¹, Gaber M. Abu El-Reash², Mohamed gaber¹ & Mohamed A. Hashem²

A new modified cellulose with diaminoguanidine (Cel-Gua) synthesized for specific recovery of Cu (II), Cd (II), and Hg (II) from the alum sample. Cellulose was silylated by 3-chloropropyltrimethoxysilane and then was modified with diaminoguanidine to obtain N-donor chelating fibers. Fourier transform-infrared spectroscopy, scanning electron microscopy, X-ray diffraction, zeta potential, electrons disperse X-ray analysis, elemental analyses (C, H and N), and thermogravimetric analysis were used for characterization. Factors influencing the adsorption were thoroughly examined. Under the optimal conditions, the Cel-Gua sorbent displayed maximum adsorption capacities of 94.33, 112.10 and 95.78 mg/g for Cu (II), Cd (II), and Hg (II), respectively. The sorption process of metal ions is equipped by kinetic model PSO and Langmuir adsorption isotherm. The calculated thermodynamic variables confirmed that the adsorption of Cu (II), Cd (II) and Hg (II) by Cel-Gua sorbent is a spontaneous and exothermic process. In our study, we used the molecular operating environment software to conduct molecular docking simulations on the Cel-Gua compound. The results of the docking simulations showed that the Cel-Gua compound displayed greater potency and a stronger affinity for the Avr2 effector protein derived from *Fusarium oxysporum*, a fungal plant pathogen (code 5OD4). The adsorbent was stable for 7 cycles, thus allowing its safe reutilization.

Keywords Silylating agent, Metal ions, Silylated cellulose, Solid phase extraction, Diaminoguanidine modified cellulose and molecular docking

Cellulose, being the most prevalent polymer in the natural world, could be sourced from various origins, including bacteria and plants. The vast bounty of chlorophyll-containing plants necessitates the utilization of chemical processes for the extraction and whitening of cellulose when producing paper and its derivatives on a large scale. On a more limited scale, as well cellulose can be derived into thin films^{1–3} and extracted from specific bacteria^{4–7}, recent studies have focused on investigating cellulose for the production of biofuel ethanol^{8–12}.

Due to the cellulose being the most and largest abundant biopolymer, additionally it has been suggested as a potential material for applications such as solid-phase extraction processes targeting for eliminating toxic metal ions in aqueous samples^{13–15}. The cellulose's capacity to perform this function is derived from the existence of hydroxyl groups in its structure, which possess the capability to participate in silylation and/or chlorination reactions¹⁶. These reactions lead to the formation of the reacting structure containing chlorine atoms appropriated throughout the polymer chain¹⁷. Silylated and/or chlorinated cellulose exhibits reactivity towards a wide array of molecules containing phosphorus, nitrogen, carboxylic acids, sulfur and other functional groups^{18,19}.

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Synthesis Of Macrocycles The Design Of Selective Complexing Agent

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