Utilization of industrial by-product fungal biomass from Aspergillus niger and Fusarium culmorum to obtain biosorbents for removal of pesticide and metal ions from aqueous solutions

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Abstract
In this work, Aspergillus niger and Fusarium culmorum cell wall by-products were chosen as microbial sources for chitin and chitosan production. Both polysaccharides were characterized by FTIR and 13C-CPMAS NMR, but GPC analysis was only performed for chitosan. SEM-EDX analysis was performed to fungal chitosan loaded with metal ions. Chitosan extracted from both fungus had low to medium molecular weight (Mw) and degree of deacetylations (DD) ranging from 65.7-83.3%. Fungal chitosan samples were intended to be used for bioremediation applications. For this purpose, two independent absorption experiments regarding pesticide Dimethoate (DM) and heavy metal ions (Al(III), As(III), Cd(II), Cu(II), Mg(II), Mn(II), Pb(II), Zn(II), Fe(II)) in a complex mixture were carried out. An experimental design considering the solution pH, contact time and chitosan physicochemical properties (DD) were performed. The highest percentage of dimethoate pesticide and selected metal ions absorption was obtained with highest DD chitosan, the contact time of 24 h, pH 6 for metals and pH 4 for pesticide, respectively. Molecular dynamics simulation studies allowed to analyze at the molecular level the chitosan-DM interaction. A higher number of h-bonds were identified as the main interactions that stabilize the affinity of the chitosan-DM complexes. Based on our results, we suggest the use of a multipurpose fungal chitosan system for water bioremediation.

Author keywords
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