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Evaluation in Vitro and in Silico of Pleurotus ostreatus Capacity to Decrease the Amount of Low-Density Polyethylene Microplastics Present in Water Sample from the Middle Basin of the Magdalena River, Colombia

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Abstract : Plastic pollution, specifically microplastics, has become a significant issue in aquatic ecosystems worldwide. The large amount of plastic waste carried by water tributaries has resulted in the accumulation of microplastics in water bodies. The polymer aging process caused by environmental influences such as photodegradation and chemical degradation of additives leads to polymer embrittlement and properties change that require degradation or reduction procedures in rivers. However, there is a lack of such procedures for freshwater entities that develop over extended periods. The aim of this study is evaluate the potential of Pleurotus ostreatus a fungus, in reducing lowdensity polyethylene microplastics present in freshwater samples collected from the middle basin of the Magdalena River in Colombia. The study aims to evaluate this process both in vitro and in silico by identifying the growth capacity of Pleurotus ostreatus in the presence of microplastics and identifying the most likely interactions of Pleurotus ostreatus enzymes and their affinity energies. The study follows an engineering development methodology applied on an experimental basis. The in vitro evaluation protocol applied in this study focused on the growth capacity of Pleurotus ostreatus on microplastics using enzymatic inducers. In terms of in silico evaluation, molecular simulations were conducted using the Autodock 1.5.7 program to calculate interaction energies. The molecular dynamics were evaluated by using the myPresto Portal and GROMACS program to calculate radius of gyration and Energies.The results of the study showed that Pleurotus ostreatus has the potential to degrade low-density polyethylene microplastics. The in vitro evaluation revealed the adherence of Pleurotus ostreatus to LDPE using scanning electron microscopy. The best results were obtained with enzymatic inducers as a MnSO4 generating the activation of laccase or manganese peroxidase enzymes in the degradation process. The in silico modelling demonstrated that Pleurotus ostreatus was able to interact with the microplastics present in LDPE, showing affinity energies in molecular docking and molecular dynamics shown a minimum energy and the representative radius of gyration between each enzyme and its substract. The study contributes to the development of bioremediation processes for the removal of microplastics from freshwater sources using the fungus Pleurotus ostreatus. The in silico study provides insights into the affinity energies of Pleurotus ostreatus microplastic degrading enzymes and their interaction with low-density polyethylene. The study demonstrated that Pleurotus ostreatus can interact with LDPE microplastics, making it a good agent for the development of bioremediation processes that aid in the recovery of freshwater sources. The results of the study suggested that bioremediation could be a promising approach to reduce microplastics in freshwater systems.

Keywords : bioremediation, in silico modelling, microplastics, Pleurotus ostreatus
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