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Study of photocatalytic degradation of some selected Dyes and other organic contaminants in water

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The present study explores the effects of various parameters such as radiation type, pH of the solution, type of photocatalyst, particle size, initial concentration of dyes and pesticide precursors, amount of H_2O_2 concentration, reaction temperature, and photocatalyst load on photocatalysis of each compound. TiO_2 nanoparticles, TiO_2 microparticles, and MnO_2 microparticles were used to compare the efficiency of the photocatalysts. Methylene Blue, Methyl Orange, and Acid Red 1 were used as synthetic dyes and p-Nitrophenol, and p-Nitroaniline as pesticide intermediates were taken as organic pollutants. The highest degradation efficiency was observed under UV irradiation compared to sunlight for all compounds. Methylene Blue at pH 8, and at pH 2 Methyl Orange, Acid Red 1, and p-Nitrophenol, and at pH 11 p-Nitroaniline showed the highest degradation. The study showed that nano TiO_2 photocatalysts had higher degrading efficiency over MnO_2 and TiO_2 microparticles. Furthermore, it was discovered that the photo-degradation efficiency of all compounds investigated was highest at low concentrations. In addition, the photodegradation efficiency of compounds was higher at high H2O2 concentrations such as 0.3 M. The results indicated that the optimal conditions for the highest degradation efficiency varied depending on the compound. Methylene blue, methyl orange, and acid red 1 showed high degradation efficiency at high temperatures like 55°C, while p-nitrophenol and p-nitroaniline showed higher degradation efficiency at 45 °C. The study further showed that all compounds displayed the highest degradation efficiency when loaded with 20 mg of TiO_2 nanoparticle photocatalyst. Overall, the study suggests that photocatalytic degradation using TiO_2 nanoparticles is a promising technology for the removal of organic pollutants from water.

Keywords:

Water contamination, Photocatalytic degradation, Organic pollutants, TiO_2 nanoparticles, Degradation efficiency

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Computational studies on flabelliferins and their bioactivities

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Flabelliferins are bioactive compounds found in palmyrah (*Borassus Flabellifer* L.). They are reported to have antiarthritic, antibacterial, anticancer, antidiabetic, anti-inflammatory, antipyretic, antioxidant activities, and effective ATPase inhibitors. The bioactive compounds of palmyrah exhibit comparable activity to selected drugs that are used to treat specific diseases such as cancer, diabetes, heart diseases, liver diseases, and Alzheimer's disease. Flabelliferin B (FB), Flabelliferin-II (F-II), and Flabelliferin-III (F-III) are such active compounds in palmyrah that have proven bioactivities against control drugs. It has been shown that FB inhibits bacterial growth and promotes wound healing. Flabelliferin-II was investigated for type 2 diabetes mellitus to inhibit dipeptidyl peptidase-4. Also, F-II inhibits the intestinal cells of the Na^+ /K^+ ATPase pump. The proliferation of cancer cells has been inhibited by F-III. Only a few monoclonal antibodies that inhibit protein cell

signaling pathways have given FDA (Food and Drug Administration) approval. The need for alternatives is quite significant due to the extremely expensive cost of monoclonal antibodies and their numerous adverse side effects. However, the class of flabelliferins is not on the list of FDA-approved drug molecules.

Computational studies on flabelliferins and their mechanism of action have been investigated using standard tools such as docking and molecular dynamic simulations (MD). The molecular docking analysis showed higher binding affinities for flabelliferins in comparison to their standard drugs *via* AutoDock Vina. Molecular dynamics have proven the functional mechanisms of each protein and ligand, determining the structural basis for specific diseases via the AMBER 20 software suite. However, explanations for some bioactive flabelliferins are yet to be discovered. Through this computational study, we have shown how flabelliferins are more effective than their comparator medications at carrying out their bioactivities, thus enabling them to be used in the pharmaceutical industry.

Keywords:
Palmyrah, Bioactivities, Flabelliferin B, Flabelliferin-II, Flabelliferin-III