Title: Mechanistic insights into methyl violet dye degradation using fish bone-derived hydroxyapatite: LC–MS/MS identification and computational analysis

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Abstract: The persistent and poisonous nature of synthetic dyes in industrial wastewater presents a significant risk to both the human health and environment. This study offers an approach for the breakdown of Methyl violet (MV) dye by utilizing fish bone hydroxyapatite (FB-HAp) that was generated from the waste of fish bones of *Mastacembelus armatus* by a thermal calcination method. The photocatalytic degradations of FB-HAp results showed 92 % degradation of MV within 240min under sunlight irradiation. In this manuscript, an eight dye degradable compounds were identified after catalytic reaction which was analyzed by LC-MS/MS. The most promising candidates are MV-3, MV-4, MV-7, and MV-9, which balance good oral absorption, non-hepatotoxicity, lack of hERG inhibition, and moderate clearance profiles with typically non-persistent, non-bioaccumulative, and only present low-to-moderate aquatic toxicity risks, according to the results of the ecotoxicity and ADMET analyses of the methyl violet degradation products. Moreover, PASS predictions data was demonstrated that the antibacterial and antiviral efficacy, particularly against picornavirus and protozoal infections, yielding promising results for antimicrobial applications. Furthermore, the proposed mechanistic pathway was figured out for degradable compounds which is a key factor for further study and environmental policy making. This study opens the door to long-lasting ways to treat wastewater by looking at the possibilities of HAp made from biowaste. It also gives us a better understanding of how it works as a photocatalyst after MV is broken down, as well as information about the impact of the degradable products.

Keywords: Fish bone hydroxyapatite, Photocatalytic degradation, Methyl violet, Degradable compounds

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