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Antibacterial, antifungal, antioxidant, and molecular docking studies of (E)-4-(1-(2-aminophenylimino)ethyl)benzene-1,3-diol

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The Schiff base, (E)-4-(1-(2-aminophenylimino)ethyl)benzene-1,3-diol (APEB) has been synthesized and characterized by different spectroscopic techniques. The Schiff base, APEB shows antibacterial and antifungal activities against a bacterium (*E. coli*) and a fungus (*C. albicans*) with an IC₅₀ value of 0.07 µg/mL and 0.06 µg/mL respectively. Clear zones have not been observed in the case of antibacterial activity but are present in the case of antifungal activity. Additionally, antioxidant potential has been evaluated through DPPH, ABTS, FRAP, CUPRAC, SOARSA, RNOSA and HFRSA, with an IC₅₀ values of 187.2 µg/mL, 5.967 ± 0.1625 µg/mL, 0.7404 µg/mL, 2.37 µg/mL, above maximum dose limit *i.e.* higher than 1000 µg/mL, 167.6 µg/mL and 9.934 µg/mL, respectively, indicating antioxidant properties. To elucidate the potential mechanisms underlying these bioactivities, molecular docking studies have been performed against the protein; PDB ID 1AI6 and 5AEZ.

Keywords: Schiff base, *o*-Phenylenediamine, Antimicrobial activity, Antioxidant activity, Molecular docking