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Synthesis, biological evaluation, ADME studies and molecular docking of 1-(3-substituted phenylisoxazol-5-yl) naphthalen-2-ol moiety with VEGFR-2 and Caspase-3 enzymes inhibitors

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In this investigation, a few isoxazole derivatives have been synthesized from the cyclization of chalcone derivative with hydroxylamine hydrochloride in a basic medium using ultrasonication. The synthesized compound has been confirmed based on ^{1}H NMR, mass spectroscopy and IR analysis. The titled compounds have been screened for their *in vivo* antimicrobial activity against *Pseudomonas aeruginosa*, *Escherichia coli*, *Staphylococcus aureus* and *Bacillus subtilis*. All compounds show excellent activity against *Escherichia coli* and *Staphylococcus aureus* bacteria. Each compound has a bioavailability score of 55%, a pain assay score of zero, complies with Lipinski's rule of five, and has high gastrointestinal (GI) absorption. Compounds **3b**, **3e**, **4b**, **4d**, and **4e** show the best docking scores with VEGFR-2 (PDB IDs: 4ASD, 4ASE) and Caspase-3 (PDB ID: 4QTX), ranging from –8.2 to –9.9 kcal/mol compared to standard curcumin and sorafenib. All the synthesized compounds have excellent docking scores. These compounds may thus be used as lead compounds in studies investigating VEGFR-2 and Caspase-3 inhibitors.

Keywords: Chalcone, Isoxazole, Antimicrobial activity, VEGFR-2, Caspase-3 enzymes

In medicinal chemistry, isoxazol