THESIS ABSTRACT

Chemical studies on some chromone derivatives with anticipated pharmaceutical applications

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Background: Heterocyclic are known to have multiple applications in particular biomedical settings. Aim: The present study reports a convenient protocol for the design and synthesis of new heterocyclic compounds incorporating 1- hydroxy-naphthyl and new angular chromones bearing allylnaphthyl fragments. Materials and Methods: The versatile precursor 2-acetyl-4- allyl-1-hydroxy naphthalene was subjected to Claisen-Schmidt condensation but the precursor 6-allyl-3-formyl-4Hbenzo[h]chromone was prepared via Vilsmeier–Haack reaction of 4-allyl-1- hydroxy-2acetonaphthone. Results: Some new compounds are considered as promising leads with dual biological activity as antibacterial and antioxidant. The isoalloxazine ring of the cofactor FAD is essential to the recognition of the compound that has proper antioxidant activity. Benzocoumarin ring is essential for the recognition of the amino acid residues. Allyl chain improves the p stacking interaction while the npropyl chain attenuates the overall interaction. Naphthyl ring needs to be substituted with a short bridge to avid the ring extended away from the pocket. The antimicrobial and anti-9quorum-sensing activities of the newly synthesized compounds showed that many compounds have good and promising activities in comparison with the reference drugs. Conclusion: Based on the computational prediction of pharmacokinetics, drug-likeness properties, biological activity, and molecular docking suggested that formyl chromone and tetracarbonyl may be potent antimicrobial drugs.

Keywords: Antimicrobial activity; Antiquorum-sensing; Docking

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