

SYNTHESIS, CHARACTERIZATION, ANTIOXIDANT ACTIVITY AND MOLECULAR DOCKING OF SOME NEW QUINOLINE HYBRIDS

BOURIA Houria ^{1*}, ALLIOUCHE Hayette ¹, CHOUITER Mohamed Imed ¹,
BENSEGUENI Rafik ^{2,3}, BELFAITAH Ali ¹

¹Laboratoire des Produits Naturels d'Origine Végétale et de Synthèse Organique. Faculté des Sciences Exactes, Campus de ChaabatErsas, Université des frères Mentouri-Constantine1. Constantine 25000, Algeria.

²Département des sciences de la matière, faculté des sciences exactes, université Chérif Messaadia - Souk Ahras.

³Laboratoire de chimie des matériaux Constantine, université des frères Mentouri Constantine 1.

Code CCO9

Email*: bouriahouria@gmail.com/houria.bouria@umc.edu.dz

Introduction & Objectives:

Nitrogen heterocycles are important structural subunits that occur widely in bioactive natural products, pharmaceuticals, cosmetics, and functional material.¹ Quinoline and its derivatives represent one of the major classes of aza-heterocycles associated with a broad spectrum of bioactivities such as antibacterial, anticancer, anticholinesterasic and neuroprotective...²

In continuation of our investigations devoted to the use of quinoline as main scaffold for the synthesis of new compounds with biological interest,^{2b,3} we aim here the synthesis, characterization, antioxidant activity evaluation and molecular docking of some new hybrids containing in their structure azinane, oxazinane and quinolone units.

Methodology (Material and methods):

The strategy adopted is based on a regioselective combination of some nucleophiles with 2,2-dicyanoquinoline oxirane under free catalyst conditions.

Results and Discussion:

The antioxidant activity was investigated using ABTS radical scavenging. All the hybrid compounds showed moderate activity comparable to that of the reference standards. Furthermore, a molecular docking study was carried out in order to estimate the cholinesterase activity. The obtained results indicate that a two target compounds inhibited both acetylcholinesterase (AChE) and Butyrylcholinesterase (BChE) enzymes through different interactions.

Conclusion:

Three new quinoline hybrids were synthesized and characterized by ¹H NMR, ¹³C NMR and IR spectral methods. The evaluation of the ABTS assay showed moderate antioxidant activities while the molecular docking study revealed that 2 compounds should have good anti-cholinesterase activity. *In vitro* evaluation will be conducted to confirm these results.

Key-words: Quinolone, Nucleophile, Hybrid compound, Antioxidant activity, Molecular docking.

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