Contents lists available at ScienceDirect

Bioorganic & Medicinal Chemistry Letters

journal homepage: www.elsevier.com/locate/bmcl

Quinolidene based monocarbonyl curcumin analogues as promising antimycobacterial agents: Synthesis and molecular docking study

Dnyaneshwar D. Subhedar [a], Mubarak H. Shaikh [a], Laxman Nawale [b], Dhiman Sarkar [b], Vijay M. Khedkar [b], Bapurao B. Shingate [a,*]

[a] Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad 431 004, India
[b] Combichem Bioresource Centre, National Chemical Laboratory, Pune 411 008, India

ARTICLE INFO

Article history:
Received 22 September 2016
Revised 5 December 2016
Accepted 4 January 2017
Available online 5 January 2017

Keywords:
Antitubercular activity
Cytotoxicity
Green protocol
Knoevenagel condensation
Molecular docking

ABSTRACT

A series of quinoline incorporated monocarbonyl curcumin analogues was efficiently synthesized using [HDBU][HSO_4] as catalyst *via* Knoevenagel type condensation and evaluated for their *in vitro* antitubercular activity against *Mycobacterium tuberculosis H37Ra* (MTB) and *Mycobacterium bovis* BCG in dormant state. The analogues **3e**, **3h**, **4a** and **4e** exhibited very good antitubercular activity. The antiproliferative activity of the analogues against MCF-7, A549 and HCT-116 cell lines was evaluated using modified MTT assay and these compounds were found to be non-cytotoxic. Molecular docking study has been carried out against *M. tuberculosis* pantothenate synthetase (MTB PS) enzyme in an effort to enhance the understanding of their action as antitubercular agents. The potency, low cytotoxicity and selectivity of these analogues support them as valid leads for further optimization.