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PII: S2405-8300(18)30101-0
DOI: 10.1016/j.cdc.2018.06.003
Reference: CDC 119

To appear in: *Chemical Data Collections*

Received date: 10 May 2018
Revised date: 5 June 2018
Accepted date: 7 June 2018

Please cite this article as: Shivarudrappa H. Pattanashetty , K.M. Hosamani , Delicia A. Barretto , Microwave assisted synthesis, computational study and biological evaluation of novel quinolin-2(1H)-one based pyrazoline hybrids., *Chemical Data Collections* (2018), doi: 10.1016/j.cdc.2018.06.003

Microwave assisted synthesis, computational study and biological evaluation of novel quinolin-2(1H)-one based pyrazoline hybrids.

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Abstract:

In the present study, an easy and efficient microwave-assisted protocol has been adopted for the synthesis of quinoline-based pyrazolines derivatives **3(a-i)**. The newly synthesized 3-(4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl)-5-phenyl-4,5-dihydropyrazole-1-carbothioamide derivatives were characterized by IR, ^{1}H, ^{13}C-NMR, Mass and Elemental analyses. *In-vitro* anti-tubercular assay of compounds **3(a-i)** has shown moderate to good activity against *M. tuberculosis* ($H_{37}Rv$) strain with MIC's ranging between 0.05 to 6.25 µg/mL. *In-silico* study further supported the observed results with higher C-score values. Further, the compounds were also screened for *in-vitro* antibacterial and antifungal activity, wherein compound **3d** and **3i** exhibited excellent antibacterial activity and compound **3g** and **3h** were found to exhibit significant antifungal activity. The predicted ADME properties suggested a good pharmacokinetic profile for the newly synthesized compounds.

Key words: Microwave synthesis; 3-acetyl-4-hydroxyquinolin-2(1H)-one; Molecular docking; Anti-tubercular activity; ADME properties.