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Synthesis of coumarin-piperazine derivatives as potent anti-microbial and anti-inflammatory agents, and molecular docking studies

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ABSTRACT

A series of novel coumarin-piperazine derivatives **(3a-3h)** were synthesized and characterized by IR, ^{1}H, ^{13}C NMR and GC-MS. All the synthesized compounds were tested by *in-vitro* anti-inflammatory and anti-microbial activity. The compounds **(3a)**, **(3d)**, **(3h)** and **(3f)** were found to be potent anti-inflammatory activity with IC_{50} values in the range of 37.15 - 61.93 µg/mL. The compounds (**3a**), (**3d**) and (**3f**) showed potent anti-microbial activity with MIC values in the range of 0.5 - 2 µg/mL. Furthermore, Molecular docking study was performed against *1AD4* enzyme of *S. aureus*, which exhibited good binding interactions and also the compounds (**3a**), (**3e**), (**3f**) and (**3h**) have higher C score values than ciprofloxacin.

Keywords:

Coumarin- piperazine derivatives; Anti-inflammatory; Anti-microbial; Molecular docking.

Graphical Abstract