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Original article

Conventional and microwave irradiated synthesis, biological activity evaluation and molecular docking studies of highly substituted piperazine-azole hybrids

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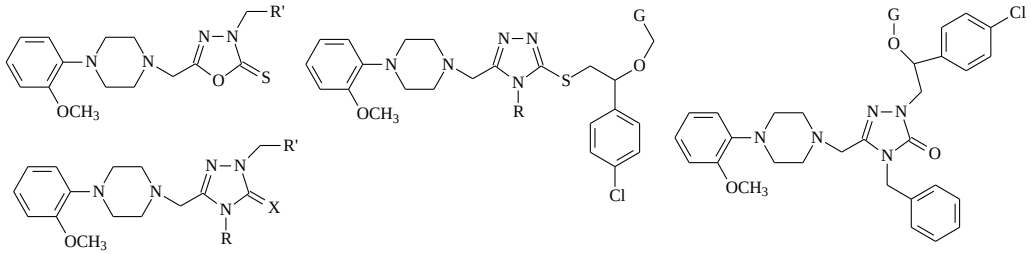
Graphical Abstract



New hybrid molecules consisting of fluoroquinolone, methoxyphenylpiperazine and azole moieties were synthesized by microwave irradiated and conventional methods. The newly synthesized compounds were screened for their antimicrobial, antiurease, antiglucosidase and antioxidant activities. Also, molecular docking studies were performed.

ABSTRACT

Azole derivatives (**3**, **6**) obtained starting from 1-(2-methoxyphenyl)piperazine were converted to the corresponding Mannich bases containing *β*-lactame or flouroquinolone core *via* a one pot three component reaction. The synthesis of conazole analogues was carried out starting from triazoles by three steps. Reactions were carried out under conventional and microwave mediated conditions. All the newly synthesized compounds were screened for their antimicrobial, enzyme inhibition and antioxidant activity, and most of them displayed good-moderate activity. Binding affinities and non-covalent interactions between enzyme-ligand complexes were predicted with molecular docking method at molecular level. Docking results complemented well the experimental results on α-glucosidase and urease inhibitory effects of the compounds. Higher binding affinities and much more interaction networks were observed for active compounds in contrary to inactive ones. It was predicted with the docking studies that triazole and anisole moieties in the structure of the synthesized compounds contributed to the stabilization of corresponding enzymes through noncovalent interactions.

Keywords:
Fluoroquinolone
1,2,4-Triazole
Microwave
Mannich reaction
Biological activity
Molecular docking