Extended Abstract

Synthesis, Spectral Characterization Antimicrobial Activity and DFT Studies of Some Tetrahydropyrimidinones [†]

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Dihydropyrimidine and tetrahydropyrimidine derivatives are pivotal heterocycles in medicinal chemistry. The reaction most often involved in the synthesis of these compounds is the multicomponent synthesis of Biginelli, which has been improved over the years [1].

Organic commercial and synthetic materials were used for the synthesis of the heterocyclic compounds. All compounds were characterized with physicochemical techniques (elemental analysis, ¹H, ¹³C, FTIR and UV-Vis spectroscopy).

In this study a series of tetrahydropyrimidinones were synthesized in two steps: 1. Biginelli synthesis [2]; 2. alkylation of intermediates from step 1. The structures of all compounds were confirmed by ¹H, ¹³C-NMR, FTIR, UV-VIS spectra and elemental analysis. A DFT analysis of molecular structure and frontier molecular orbitals HOMO-LUMO was performed using the GAMESS 2012 software [3–6]. All compounds were evaluated by qualitative and quantitative methods against a panel of selected bacterial and fungal strains.

It was found that the presence of nucleophilic group and symmetry of the molecule are advantages for a high antimicrobial activity.

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