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Synthesis, biological activity and DFT studies of new hydropyrimidine compounds

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A series of the dihydropyrimidinones was obtained by the Biginelli condensation using ZnO nanoparticles as catalyst. A new series of compounds was obtained by alkylation of the dihydropyrimidinones with different halogenated compounds (Fig. 1). The structures of all compounds were confirmed by 1H, 13C-NMR, FTIR, UV-VIS spectra and elemental analysis. All derivatives were evaluated by qualitative and quantitative methods against a panel of selected bacterial and fungal strains. A DFT analysis of molecular structure and frontier molecular orbitals HOMO-LUMO was performed using the GAMESS 2012 software. Antimicrobial activity of the synthesized compounds (Fig. 2) was corelated with electronic parameters (chemical hardness, electronic chemical potential, global electrophilicity index), Mullikan atomic charges and geometric parameters of the tetrahydropyrimidines calculated with GAMESS. It has been found that the presence of nucleophilic group and the symmetry of the molecule are advantages for a high antimicrobial activity.

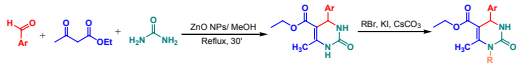

Figure 1. The synthesis of the compounds

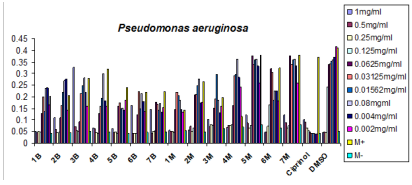

Figure 2. Antimicrobial activity of tested compounds against Pseudomonas aeruginosa

Biography

Maria Marinescu has completed his PhD from University of Bucharest. He is Assistant Professor in the department of Organic Chemistry, Biochemistry and Catalysis, a premier research organization. He has published more than 30 papers in reputed journals.

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