One-pot synthesis, theoretical study and antimicrobial activity of 5,5′-(1,4-phenylenebis-(methanylylidene))Bis(3-Aryl(Alkyl)-2-thioxoimidazolidin-4-one) derivatives

Abstract

A simple, facile, and convenient practical method for the one-pot synthesis of pharmaceutically interesting 5,5`-(1,4-phenylenebis-(methanylylidene))bis-thiohydantoins via a three-component condensation reaction of terephthalaldehyde, α-amino acids and isothiocyanates had been developed. The *S*-alkylated derivatives **6a** and **6b** were obtained by the alkylation of the bis-thiohydantoins **4a** with methyl iodide and/or benzyl chloride in a basic media. The molecular structures of the synthesized compounds were confirmed by their elemental analyses and spectral data (IR, ^{1}H, ^{13}C NMR and MS). The assignment of more stable *Z*- or *E*-isomers as the major form of **4a**, **6a,** and **8a** was investigated by DFT calculations at B3LYP/6-31+G* level. Some of the prepared compounds were screened for their *in-vitro* antimicrobial activity. Compounds **4a**, **6 b**, **8 b** and **8c** exhibited low antibacterial activity against gram-positive bacteria *Bacillus cereus*. (5*Z*,5′*Z*)-5,5′-(1,4-Phenylenebis(methanylylidene))bis(3-benzyl-2-thioxoimidazolidin-4-one) (**4b**) exhibited good fungicidal activity against *Fusarium oxysporum*.