Synthesis and Characterization of Compounds Obtained by Biginelli-Type Reaction: 4-(4-methoxyphenyl)-6-phenyl-3,4-dihydropyrimidine-2(1*H*)-thione and of 4-(2-bromophenyl)-6-phenyl-3,4-dihydropyrimidine-2(1*H*)-thione.

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Introduction

The present work shows an efficient route to synthesize thiones with free five position, a group of compounds with structure related to the Monastrol few investigated due to a lack of synthetic alternatives. The compounds synthesized are possible candidates to be used like drugs with anticancer activity.[1] The synthesis of 4-(2-bromophenyl)-6-phenyil-3,4-dihydropyrimidine-2(1*H*)-thione and of 4-(4-methoxyphenyl)-6-phenyl-3,4-dihydropyrimidine-2(1*H*)-thione were carried out using a multicomponent reaction of Biginelli-type,[2] once only Biginelli reaction does not present synthetic efficiency to the desired compound. The reaction was catalyzed by hydroxide sodium in two steps: the first one that pass for the formation of chalcone as an intermediate of reaction, once obtained the intermediary follow the second step in order to obtain the final product under microwave heating conditions. The compounds were characterized by nuclear magnetic resonance (NMR) and Gas Chromatography Mass Spectrometry (GCMS).

Results and Discussion

The intermediary obtained in the first step of reaction was identified by thin layer chromatography (TLC). The chalcone having bromo and methoxy in its structure showed yielding of 87% and 80%, respectively and the respective thiones 75% and 83%. The NMR analysis presented to the bromo thione a singlet at ŭ = 7,9 to the hydrogen from amine group (1); a doublet at ŭ = 7.6 corresponding to the second amine group (2); a doublet at ŭ = 5.348 assigned to hydrogen from Csp^3 (3), a singlet at ŭ = 5.6 to the hydrogen Csp^2 (4); doublet at ŭ = 7.5, ŭ = 7.4, ŭ = 7.2 that probably corresponds to hydrogen from aromatic (Fig. 1A). For the second compound, methoxy-thione, the NMR analysis showed the following characteristics: a singlet at ŭ = 6.9 to the hydrogen from amine group (1); a doublet at ŭ = 7.2 corresponding to the second amine group (2); a singlet at ŭ = 5.2 assigned to hydrogen from Csp^2 (3), a singlet at ŭ = 5.6 to the hydrogen Csp^2 (4); multiplets at ŭ = 7.4 and ŭ = 7.3 that 1). The GCMS analysis of methoxy compound resulted in the mix of two products. The first had 29% and the second, methoxy thione, with 71%. The later showed one intense peak mass/charge (m/z) equal to 296.1. This result is exactly the molecular formula of $C_{17}H_{16}N_2SO$ with molar mass of 296.1 g/mol.

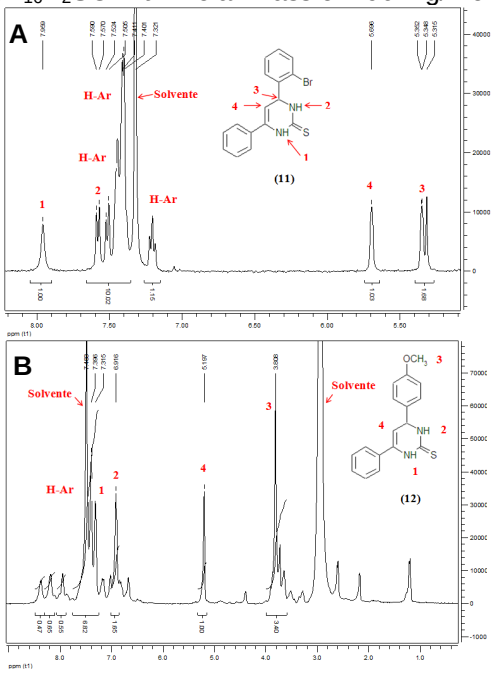

Figure 1 - NMR spectrum of: **A**) bromo-thione and **B**) methoxy thione.

Conclusions

According to results obtained by NMR and GCMS the use of Biginelli-type reaction was considerably efficient as well easy, fast and cheap of the point of view to prepare dihydropyrimidinethiones with free five position.

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