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Catalytic Synthesis and Characterization of N-(4-(Tert-Butyl) Benzyl)-1-(4-Tert-Butyl) Phenyl)-N-Methyl Methanaminium Chloride from Tert-Butyl Benzyl Derivatives

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Abstract : Butenafine (N-4-tert-butyl benzyl-N-methyl-1-naphthylene methylamine hydrochloride) is a benzylamine antimycotic (antifungal) agent that has a broad spectrum of action. The quest for improved antimycotic action brought about many research on the structure-activity properties of butenafine in relation to other antifungal agents. Of all those research, only little or no effort was recorded on the substituents attached to the aromatic systems in butenafine. In this research, N-(4-(tert-butyl) benzyl)-1-(4-tert-butyl) phenyl)-N-methyl methanaminium chloride, which is a butenafine analogue was synthesised from tert-butyl benzyl derivatives, by reductive amination using various solvents through a direct approach, where 1,2-dichloroethane gave the best solvent action at 40 °C (Yield: 75%) and of all the reducing agents used, sodium borohydride was found to give the best reducing action in the presence of silica chloride at room temperature (Yield: 50%). Characterization of the compound by 1H NMR showed a singlet peak of 18 hydrogen atoms with a chemical shift at 1.3-1.5 ppm for the presence of 6 methyl groups in the two tert-butyl substituents, the 13C NMR also indicated the presence of the two tert-butyl substituents by the peak with a chemical shift at 31-32 ppm for the six methyl carbon atoms, the IR indicated the presence of a tertiary ammonium ion by a strong band at 2460 cm-1 and finally the EIS-MS confirmed the molar mass of the compound by a mass to charge ratio of 324.2693. These results suggested that the target molecule was actually synthesised and therefore, 1,2-dichloroethane is a good solvent for this synthesis, and the most suitable reducing agent is sodium borohydride.

Keywords : antimicrobial agents, antimycotic agents, butenafine, chemotherapeutic agents, semisynthetic agents
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