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Synthesis of 1,4-naphthoquinone derivatives using 1,3-dipolar cycloaddition and Sonogashira reactions

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ABSTRACT: Naphthoquinones are known according to their important bio-activities, such as their antitumoral and topoisomerase inhibition properties. From 2-azido (3) or 2,3-diacetylene-1,4-naphthoquinone (4) it was possible to obtain triazole derivatives (naphthoquinonic). This work describes the synthesis of two novel molecules, with triazole groups linked to 1,4-naphthoquinone using the 1,3-dipolar cycloaddition and Sonogashira reactions. The synthetic strategy followed two routes (Scheme 1). First, we synthesized the 2-bromo-1,4-naphthoquinone (2, yield 98%) by using Br₂ and CH₃CO₂H, and then used it to obtain 2-azido-1,4-naphthoquinone (3, yield 62%) from compound 1, along with ethanolic solution (reflux) and NaN₃. Finally, we prepared 1,2,3-triazole compounds (4ₐ, b) by 1,3-dipolar cycloaddition, involving compound (3) and terminal acetylenes (phenylacetylene, a) and glycoside (b) using Cu(OAc)₂ and ascorbate, under argon atmosphere. During the second step, 2,3-dibromo-1,4-naphthoquinone was prepared using Br₂/CH₂Cl₂ at room temperature. From compound (5) it was possible to synthesize (6), catalyzed by Pd(PPh₃)₂Cl₂/CuI/E₃N, under argon atmosphere, in 40% yield. The 1,3-dipolar cycloaddition reactions involving 2-azido-1,4-naphthoquinone (3) and alkynes (a, yield 23% and b, yield 30%) were conducted using the solvent system, (1:1) trec-BuOH/H₂O/reflux/ 20 mol% of Cu(OAc)₂ and sodium ascorbate, under stirring during 24 hours. The reaction involving 2,3-dibromo-1,4-naphthoquinone (5, yield 65%) and phenylacetylene was prepared using the solvent mixture (2:1) DMSO/CHCl₃ and catalytic amount of CuI/Pd(PPh₃)₂Cl₂. The final products were characterized by elemental analysis and spectrometric techniques (IR, NMR ¹H and ¹³C). Two novel triazole compounds were synthesized from naphthoquinones by 1,3-dipolar cycloaddition from suitable 1,4-naphthoquinones obtained by Sonogashira couplings.

Keywords: 1,4-naphthoquinone; cycloaddition 1,3-dipolar; Sonogashira coupling

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