REACTION OF 4,6-DIAMINO-2-MERCAPTOPYRIMIDINE WITH ALKYL HALIDE

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https://doi.org/10.5281/zenodo.17336473

Pyrimidine derivatives are among the most important compounds in medicinal chemistry and pharmaceutics [1], possessing a wide range of biological activities, including antidiabetic [2], anti-inflammatory [3], anticancer [4], antibacterial [5], antihypertensive, as well as antifungal and antitubercular properties [6].

The aim of this work is to obtain new potential classes of biologically active compounds through the synthesis of an S-alkylated derivative of 4,6-diamino-2-mercaptopyrimidine – 2-{(n-pentylthio)}pyrimidine-4,6-diamine. According to the literature, such derivatives may exhibit antibacterial, antifungal, antitumor, and insecticidal properties. Therefore, their synthesis and subsequent evaluation of biological activity are the main objectives of this study.

Synthesis of 2-{(n-pentylthio)}pyrimidine-4,6-diamine

A two-necked round-bottom flask equipped with a reflux condenser was charged with 50 mg (0.351 mmol) of DAMP, which was dissolved in 5.0 mL of MeOH. Then, 0.35 mL of 1.0 N NaOH solution (0.35 mmol) was added, and the reaction mixture was stirred at room temperature for 1 h, resulting in the formation of a yellowish compound. The obtained product was dissolved in 5.0 mL of DMF. To this solution, 0.052 mL (density 1.215 g/mL, 0.421 mmol) of n-pentyl bromide was added dropwise, and the mixture was stirred at 50 °C for 16 h under magnetic stirring. The reaction progress was monitored by TLC. After completion, the mixture was cooled to room temperature, and the solvent was removed under reduced pressure using a rotary evaporator. The crude product was purified by extraction with chloroform and water.

Yield: 50.69 mg (68%). Product: 2-{(n-pentylthio)}pyrimidine-4,6-diamine – brown solid. m.p.: 92–93 °C. Rf: 0.62 (system: ethyl acetate:hexane 1:2). HRMS (ESI-TOF): m/z [M+H$^+$] calcd. for $C_9H_{17}N_4S^+$ = 213.1168; found = 214.1236.

Thus, the reaction of DAMP with n-pentyl bromide afforded 2-{(n-pentylthio)}pyrimidine-4,6-diamine in 68% yield. The physical and spectral properties of the product were determined.