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9-Methyl-3-phenyl-4*H*,6*H*--[1,2,4]triazino[5,4-b][1,3,4]thiadiazin-6-one

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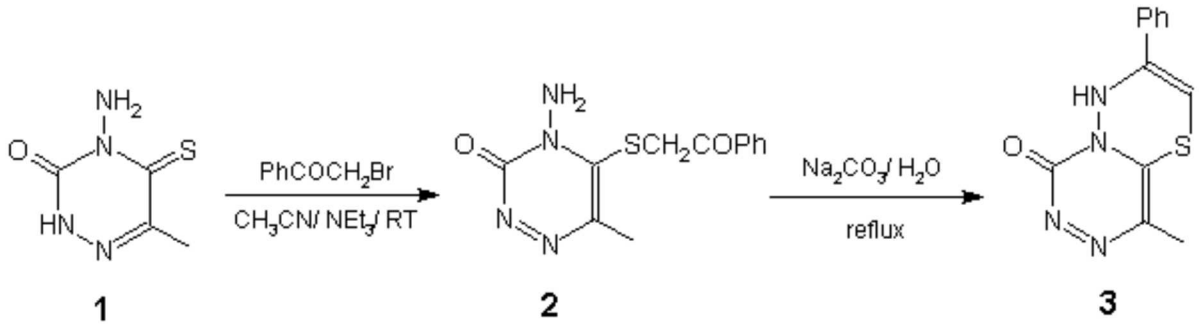

4-Amino-6-methyl-5-thio-1,2,4-triazin-3-one **1** was reacted with phenacyl bromide in the presence of triethylamine in acetonitrile to give the corresponding 5-phenacylthio derivative **2**. The latter was refluxed in aqueous solution of sodium carbonate to afford a novel heterocyclic system **3** (Scheme). Compound **1** (0.316 g, 2 mmol) was dissolved in a solution of CH_3CN (10 mL) and triethylamine (2 mL). To this solution phenacyl bromide (0.4 g, 2 mmol) was added. The reaction mixture was stirred at room temperature for 5 hrs. The solvent was evaporated to dryness and the residue was crystallized from methanol to afford **2**. Compound **2** was refluxed in a solution of sodium carbonate (0.5 g in water (6 mL)) for 2 hrs. The solution was neutralized by addition of 2N HCl and extracted with $CHCl_3$. The solvent was evaporated to dryness and the residue was directly subjected to column chromatography ($CHCl_3$:MeOH; 98:2) to afford **3**.

Selected Data for **2**. Yield: 71%, mp.: 202-3° C, ^{1}HNMR (DMSO, d_6) d, 2.3(s, 3H, Me), 5.6(s, 2H, NH_2, exchangeable with D_2O), 7.6 and 8.8 (m, 5H, Ph). IR, $\tilde{\nu}$ (KBr disc): 3400, 3350, 1690, 1580, 1400, 1210 cm^{-1}, M.S., m/z, M+, 276(65), 275(8), 105(58.5), 104(100), 103(63), 89(70), 80(74), 77(63).

Selected Data for **3**. Yield: 50%, mp.: 230-2° C, ^{1}HNMR (DMSO, d_6) d, 2.3(s, 3H, Me), 5.3(s, 2H, NH, exchangeable with D_2O), 5.4(s, 1H, =CH), 7.2-8.3(m, 5H, Ph). IR, $\tilde{\nu}$ (KBr disc): 3490, 1690, 1410, 800 cm^{-1}, M.S., m/z, M+, 258(3), 255(11), 103(100), 71(44), 42(41).

Reference

1. Heravi, M.M.; Rajabzadeh, Gh.; Rahimizadeh, M.; Bakavoli, M.; Ghassemzadeh, M. *P, S, Si and Related Elements*, submitted, **2000**.

Sample Availability: Available from the authors and from MDPI.