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A CONVENIENT METHOD FOR THE SYNTHESIS OF 4,6,7,8-TETRAHYDROPYRROLO[1,2-*a*]THIENO-[2,3-*d*]PYRIMIDIN-4-ONES

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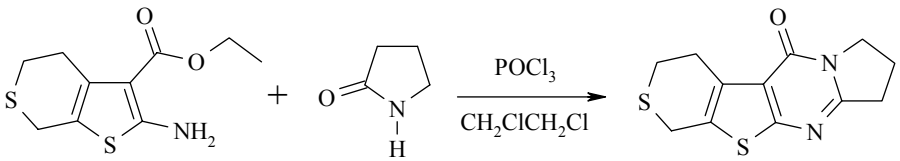
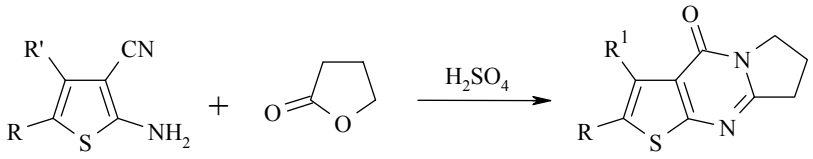
Keywords: butyrolactone, 2-amino-3-cyanothiophenes, thieno[2,3-*d*]pyrrolo[1,2-*a*]pyrimidin-5-ones.

A method is known for preparing 3,4,5,7,8,9-hexahydro-1H-pyrrolo[1,2-*a*]thiopyrano[4',3':4,5]-thieno[2,3-*d*]pyrimidin-5-one (**1**) by treatment of the 2-amino-3-ethoxycarbonylthiophene derivative **2** with pyrrolidone *via* refluxing in dichloroethane in the presence of phosphorus oxychloride [1]:



2 **1**

We propose the preparation of a pyrrolothienopyrimidinone structure (compound **3**) by another route *via* the reaction of the 2-amino-3-cyanothiophene derivative **4** with an excess of butyrolactone in the presence of sulfuric acid:



4a,b **3a,b**

3, 4 a R = COOEt, R^1 = Me; **b** R + R^1 = $(CH_2)_4$

IR spectra were taken on a Specord-M80 instrument as a suspension in vaseline oil and ^{1}H NMR spectra on a Bruker AM-300 instrument (300 MHz) using DMSO and with TMS as internal standard. Mass spectra were recorded on a Varian CH-6 instrument (EI, 70 eV).

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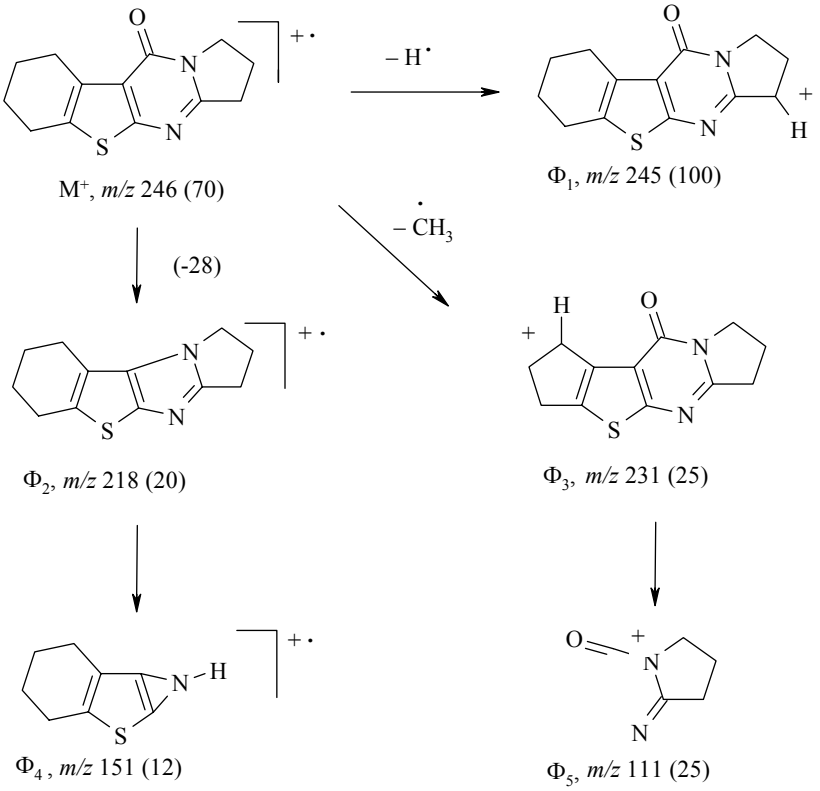
Ethyl 3-methyl-4-oxo-4,6,7,8-tetrahydropyrrolo[1,2-*a*]thieno[2,3-*d*]pyrimidine-2-carboxylate (3a). Yield 52% with mp 270°C (from a mixture of ethyl acetate and petroleum ether). IR spectrum, ν, cm^{-1}: 1745 (COOEt); 1635 (amide). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 1.32 (3H, t, *J* = 6.7, $OCH_2C\underline{H}_3$); 2.31 (2H, m, 7-CH_2); 2.82 (3H, s, 3-CH_3); 3.01 (2H, t, *J* = 7.2, 8-CH_2); 4.15. (2H, br s, 6-CH_2); 4.31 (2H, q, *J* = 6.7, $OC\underline{H}_2CH_3$). Found, %: 56.23; H 5.24; N 9.91. $C_{13}H_{14}N_2O_3S$. Calculated, %: C 56.10; H 5.07; N 10.07.

1,2,3,5,6,7,8,9-Octahydrobenzo[4,5]thieno[2,3-*d*]pyrrolo[1,2-*a*]pyrimidin-5-one (3b). Yield 57% with mp 290°C (decomp.) (from a mixture of ethyl acetate and petroleum ether). IR Spectrum, ν, cm^{-1}: 1637 (amide). ^{1}H NMR Spectrum, δ, ppm (J, Hz): 1.73-1.81 (4H, m, 7-CH_2 and 7-CH_2); 2.23-2.33 (2H, m, 2-CH_2); 2.72-2.73 (2H, m, 6-CH_2); 2.87-2.88 (2H, m, 9-CH_2); 2.97 (2H, t, *J* = 7.47, 1-CH_2); 4.08 (2H, t, *J* = 6.99, 3-CH_2). Mass spectrum, *m/z* (I_{rel}, %): 246 (70), 245 (100), 231 (25), 218 (20), 151 (12), 111 (25), 91 (25), 65 (15), 43 (20). Found, %: C 63.66; H 5.75; N 11.45, $C_{13}H_{14}N_2OS$. Calculated, %: C 63.39; H 5.73; N 11.37.

The fragmentation of the molecular ion for compound **3b** is characterized by three decomposition routes:



REFERENCES

1. F. Sauter, J. Froehlich, and E. R. Ahmed, *Monatsh. Chem.*, **127**, 319 (1996).