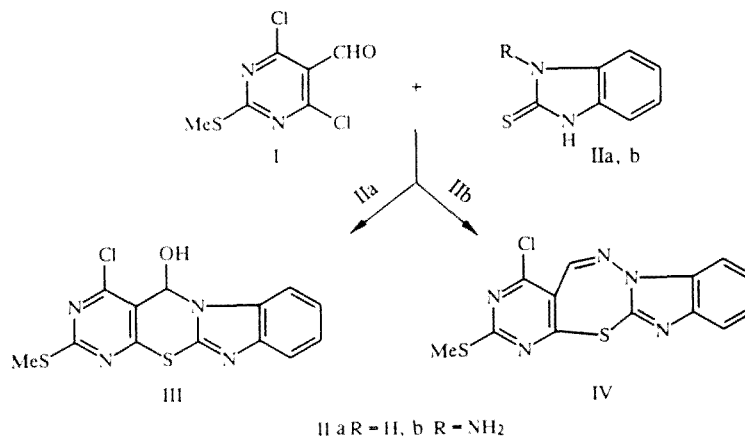


LETTERS TO THE EDITOR

5H-BENZIMIDAZO[2',1':2,3][1,3]THIAZINO[6,5-d]-PYRIMIDINE AND BENZIMIDAZO[2,1-b]PYRIMIDO[5,4-f][1,3,4]THIAZEPINE. NOVEL HETEROCYCLIC SYSTEMS

A. Brukshtus, T. Sadauskas, and S. Tumkyavichyus

In continuation of work to synthesize pyrimidine and benzimidazole heterocycles [1-3], being of interest in a planned search for biologically active materials, we report here the synthesis of the first members of the novel heterosystems 5H-benzimidazo[2',1':2,3][1,3]-thiazino[6,5-d]pyrimidine and benzimidazo[2,1-b]pyrimido[5,4-f][1,3,4]thiadiazepine. The basis of the reaction is a cyclocondensation between 2-methylthio-4,6-dichloropyrimidine-5-carboxaldehyde (I) and benzimidazoline-2-thione (IIa) or 1-aminobenzimidazoline-2-thione (IIb).



Hence, a mixture of I [4] (2.24 mmole) and IIa or IIb [5] (2.24 mmole) in DMF (10 ml) was heated for 3 h at 35-50°C (in the case of the synthesis of IV, 12 h). After cooling, the precipitate was filtered and recrystallized to give III or IV respectively.

5-Hydroxy-2-methylthio-4-chloro-5H-benzimidazo[2',1':2,3]-[1,3]thiazino[6,5-d]pyrimidine (III). Yield 71%, mp 234-236°C (from DMF-EtOH). ¹H NMR spectrum (DMSO-D₆): 2.57 (3H, s, SCH₃), 7.17 (1H, s, CH), 7.37 (2H, m, aromatic protons), 7.76 (2H, m, aromatic protons). Found, %: C 46.64, H 2.62, N 16.63. C₁₃H₉ClN₄OS₂. Calculated, %: C 46.35, H 2.69, N 16.63.

2-Methylthio-4-chlorobenzimidazo[2,1-b]pyrimido[5,4-f][1,3,4]thiadiazepine (IV). Yield 54%. Mp 196.5-197.5°C (from EtOH). ¹H NMR spectrum (CF₃COOD): 2.29 (3H, s, SCH₃), 7.41 (4H, br s, aromatic protons), 8.57 (1H, s, N=CH). Found, %: C 46.99, H 2.23, N 21.06. C₁₃H₈ClN₅S₂. Calculated, %: C 46.77, H 2.41, N 20.98.

The IR spectra of III and IV show the absence of absorption bands for CO and amino groups typical of starting I, IIa or IIb. The IR spectrum of III shows a broad band for OH at 3100 cm⁻¹.

REFERENCES

1. S. Tumkevicius, J. Prakt. Chem., **336**, 160 (1994).
2. S. Tumkevicius, Liebigs Annalen, p. 1703 (1995).
3. A. B. Brukhshtus, V. N. Garalene, A. R.-R. Sirvidite, and V. K. Daukshas, Khim.-farm. Zh., No. 6, 24 (1994).
4. A. A. Santilli, D. H. Kim, and S. V. Wanser, J. Heterocycl. Chem., **8**, 445 (1971).
5. O. V. Kryshalyuk, V. V. Kuz'menko, and A. F. Pozharskii, Zh. Org. Khim., **28**, No. 11, 1328 (1992).