

THE SYNTHESIS OF PYRAZOLO[3,4-d]PYRIMIDINE AND PYRIMIDO[4,5-e][1,3,4]-  
THIADIAZINE DERIVATIVES FROM 6-HYDRAZINOURACILS

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1,3-Dialkyl-6-hydrazinouracils (I) reacted with alkyl-, aryl-, or acyl isothiocyanates to yield 6-(4-substituted thiosemicarbazido)uracils (II), which were heated in dimethylformamide (DMF) to afford 3-substituted aminopyrazolo[3,4-d]pyrimidines (III). III was also obtained directly by the reaction of I with isothiocyanates in DMF at an elevated temperature.

Oxidation of II with N-chlorosuccinimide (NCS) in chloroform afforded 2-substituted aminopyrimido[4,5-e][1,3,4]thiadiazines (IV) as a new ring system in good yield. Heating of IV resulted in the ring contraction to III. On the other hand, oxidation of II with bromine in place of NCS afforded [1,2,3]thiadiazolo[3,4-d]pyrimidines (V) or N,N'-dialkyl-1,3,9,11-tetramethyldipyrimido[4,5-e:4',5'-k][1,7,3,4,9,10]dithiatetraazacyclododecine-2,4,6,10,12,14[1H,3H,9H,11H]hexanone-6,14-diimines (VI) depending on the reaction conditions used. V was obtained both by treatment of I with thionyl chloride and by treatment of IV with bromine. The latter reaction indicated that IV was the intermediate of the formation reaction of V from II. The mechanisms of these reactions are also discussed.

